

# PM011 – 03 January 2024

## Update on PINNs

Application to Urban Wind Field Dispersion Studies

# Script Version v4

- 1) PINN is now completely customizable – customizable input and output parameters, batch normalization, dropout rate, neuron number, number of hidden layers – all options in the config file (PM007)
- 2) Saving of all the losses (not just the total loss) (PM007)
- 3) Plotting of loss vs epochs now automatic (PM007)
- 4) Boundary conditions – relaxed no slip condition included (PM007)
- 5) New angles included (PM007)
- 6) Smaller batch sizes (I disagree) – customizable from config file (PM007)
- 7) Testing and Predicting Loss during training phase (PM008)
- 8) Inlet Boundary Conditions added (PM008)
- 9) Inlet Boundary for the Z-direction made to follow a log equation (PM009)
- 10) Debugged for no slip loss BC (PM009)
- 11) Activation function updated to an exponential linear unit instead of ReLu {arXiV: 1511.07289} (PM0010)
- 12) **Entire script revamped for optimisation → Script Version v5**
- 13) **Adaptive Weighting Scheme implemented (PM011)**
- 14) **Moving averages for stopping condition implemented (PM011)**
- 15) **Amount of data to be considered for data loss is configurable (PM011)**
- 16) **Plotting divergence implemented (PM011)**
- 17) **When running in batch mode, each batch now contains a fair representation of all angles in the training phase (PM011)**
- 18) **Script has been modified for TPU use for data loss only (PyTorch → Tensorflow) (PM011)**

# Script Version v5 – Adaptive Weighting

- 1) Adaptive weighting based on training progress is a dynamic approach to fine-tuning the contribution of different components in a composite loss function.
- 2) This method acknowledges that the relative importance of various aspects of the model's performance may change over the course of training.
- 3) Initially, in many learning scenarios, it is beneficial to give more weight to data fidelity. This means prioritizing the accuracy of the model's predictions in alignment with the available data, which is critical for the model to capture the underlying patterns and relationships. Such an emphasis is crucial in the early stages of training, where the model is still learning the basic structure of the data and is far from converging to a suitable parameter configuration.
- 4) As training progresses, the model's understanding of the data improves, and it starts capturing the fundamental trends and patterns. At this stage, it becomes increasingly important to ensure that the model does not overfit to the training data.
- 5) This is where the focus can gradually shift towards enforcing other constraints, such as physical laws or boundary conditions.
- 6) These constraints often represent critical knowledge about the underlying system or environment and are crucial for the model's ability to generalize well to unseen data.
- 7) For instance, in physics-informed neural networks, as the training evolves, increasing the weight of the physics-based loss component ensures that the model's predictions adhere to physical laws, enhancing its extrapolation capabilities.
- 8) Implementing adaptive weighting requires careful consideration of how the weights are initialized and how they are adjusted at each step or epoch.
- 9) This involves choosing appropriate schedules or performance metrics and tuning the rate of change of weights.
- 10) The goal is to strike a balance where the model neither underfits nor overfits any particular aspect of the loss function, allowing for a harmonious and effective learning process.

# Script Version v5 – Adaptive Weighting

```
def adaptive_loss(config, loss_dict, epoch, max_epochs):
    # Extract individual loss components from the dictionary
    data_loss = loss_dict.get('data_loss', 0)
    inlet_loss = loss_dict.get('inlet_loss', 0)
    no_slip_loss = loss_dict.get('no_slip_loss', 0)
    cont_loss = loss_dict.get('cont_loss', 0)
    momentum_loss = loss_dict.get('momentum_loss', 0)

    # List of individual loss components
    loss_components = [data_loss, inlet_loss, no_slip_loss, cont_loss, momentum_loss]

    initial_weight_data = config["loss_components"]["adaptive_weighting_initial_weight"]
    final_weight_data = config["loss_components"]["adaptive_weighting_final_weight"]

    weight_data = adaptive_weighting(epoch, max_epochs, initial_weight_data, final_weight_data)

    # Check for active physical loss components (non-zero)
    active_physical_losses = [loss for loss in loss_components[1:] if loss != 0]
    num_active_physical = len(active_physical_losses)

    # Calculate the weight for each physical loss component
    weight_physical = (1 - weight_data) / num_active_physical if num_active_physical > 0 else 0

    # Calculate total loss with adaptive weighting
    total_loss = weight_data * data_loss if data_loss != 0 else 0
    for physical_loss in active_physical_losses:
        total_loss += weight_physical * physical_loss

    return total_loss
```

# Script Version v5 – Moving Average Stopping Condition

- 1) The Simple Moving Average (SMA) is the arithmetic mean of a set number of data points over a specific period.
- 2) It is calculated by adding up a set of values and then dividing by the count of those values.

$$\text{SMA} = \frac{1}{N} \sum_i P_i ; i=[0,N]$$

where N is the number of time periods (epochs) and  $P_i$  are the data points.

- 3) Characteristics:
  - 3.1) Easy to calculate and interpret.
  - 3.2) Useful for identifying overall trends.
  - 3.3) Treats all data points equally.

# Script Version v5 – Moving Average Stopping Condition

```
sma = 0
sma_window_size = 1000
sma_threshold = 1e-5
consecutive_sma_threshold = 10
recent_losses = collections.deque(maxlen=sma_window_size) #deque - stays a constant maximum size by dropping the 0th element after maximum size has been reached
consecutive_sma_count = 0

recent_losses.append(current_loss.cpu().detach().numpy()) #append the current loss
if len(recent_losses) == sma_window_size: #if it reaches maximum size
    sma = sum(recent_losses) / sma_window_size # compute the SMA
    if sma < sma_threshold:
        consecutive_sma_count += 1
        if consecutive_sma_count >= consecutive_sma_threshold:
            print(f"SMA of loss below {sma_threshold} for {consecutive_sma_threshold} consecutive epochs at epoch {epoch}. Stopping training... time: {(get_time_elapsed(start_time, time_passed)):.2f} seconds")
            early_stop = True
            break
    else:
        consecutive_sma_count = 0
else:
    consecutive_sma_count = 0
```

# Scripts v4 – Preliminary Results

# Some Parameters

Infinite epochs - instead the criteria for stopping is  $\text{loss}_{\{n\}} - \text{loss}_{\{n-1\}} < \epsilon$  for 10 consecutive epochs where n is the epoch number and  $\epsilon = 1E-5$  (user defined)

128 Neurons for the PINN unless otherwise specified

We have the data for 13 angles, [0, 15, 30, 45, 60, 75, 90, 105, 120, 135, 150, 165, 180] in degrees

We concatenate the data for angles = [0, 15, 30, 45, 60, 75, 90, 105, 120, 135, 150, 165, 180] and then take 99% of the dataset with random seed = 42 for training and 1% for testing

By using 99% of the whole dataset we hope to make the NN learn about wind angle such that the parameters become functions of the wind angle

Then using the trained neural network we predict the data for angle = 135

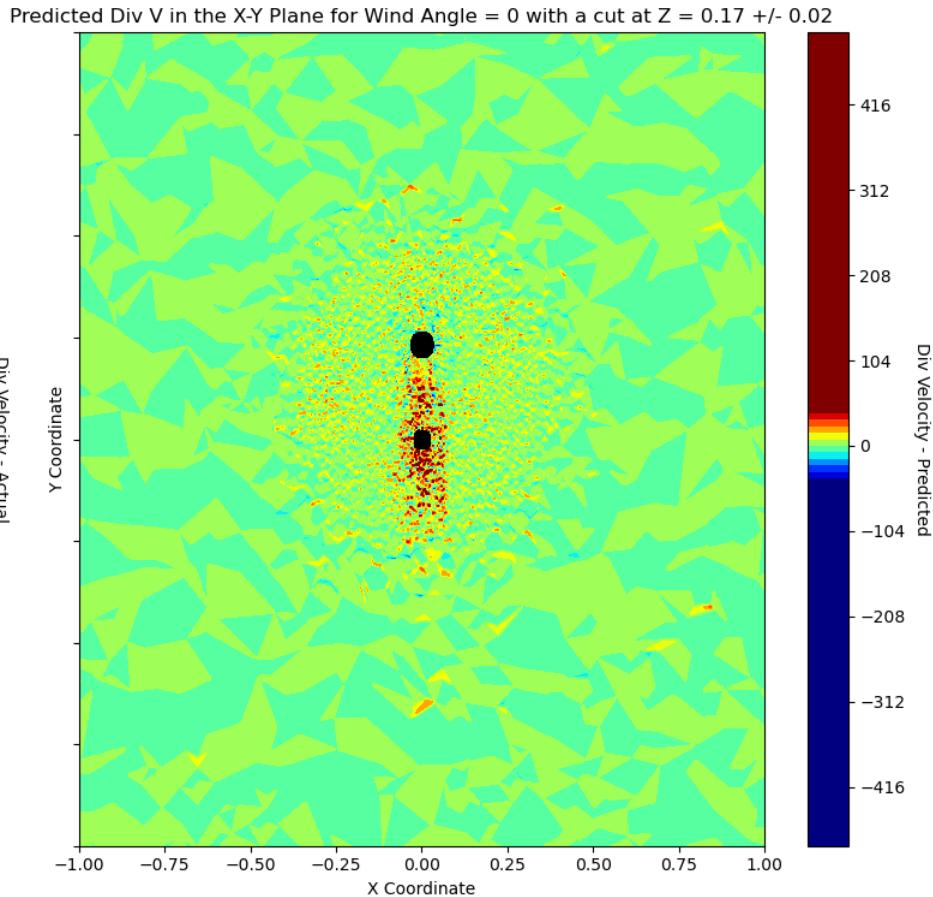
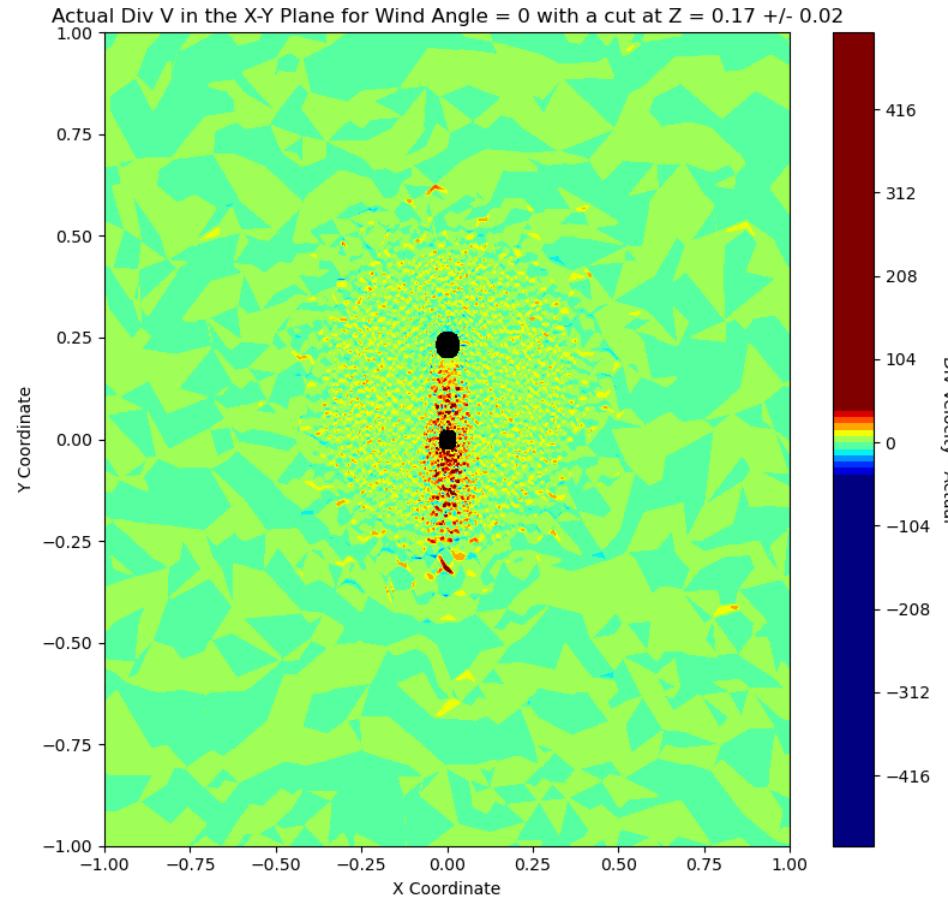
For this run, we will only have input parameters to be [X, Y, Z,  $\cos(\theta)$ ,  $\sin(\theta)$ ] and the output parameters will be [U, V, W]

Progress so far - Data Loss Only  
Standard Normal Scalar  
(Adam Optimizer)

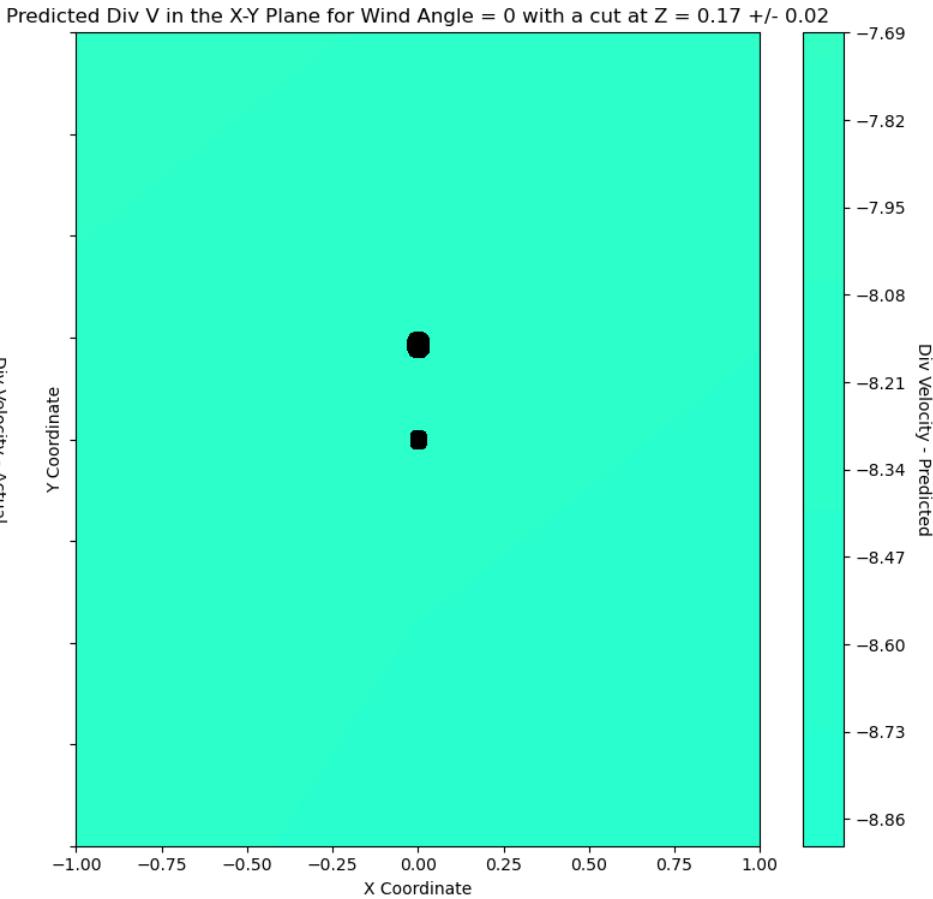
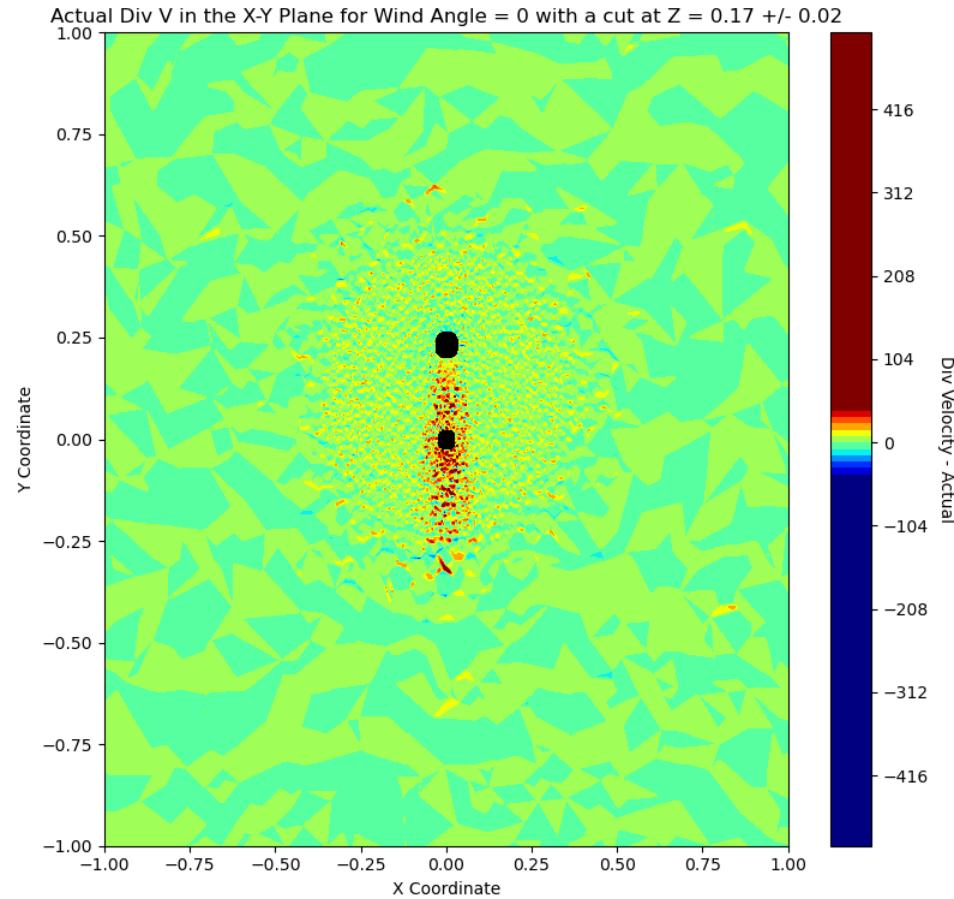
Threshold = 1E-5 (28365 Epochs, not completed), GPU Laptop

Scripts v4 – Plotting Divergence

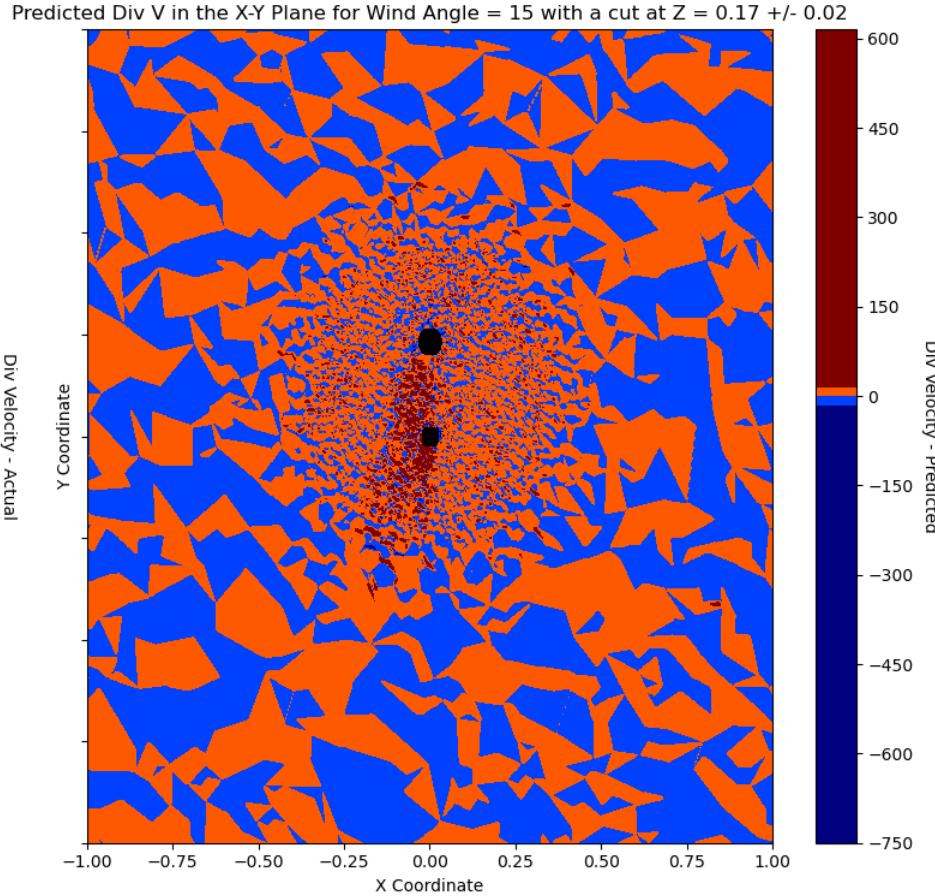
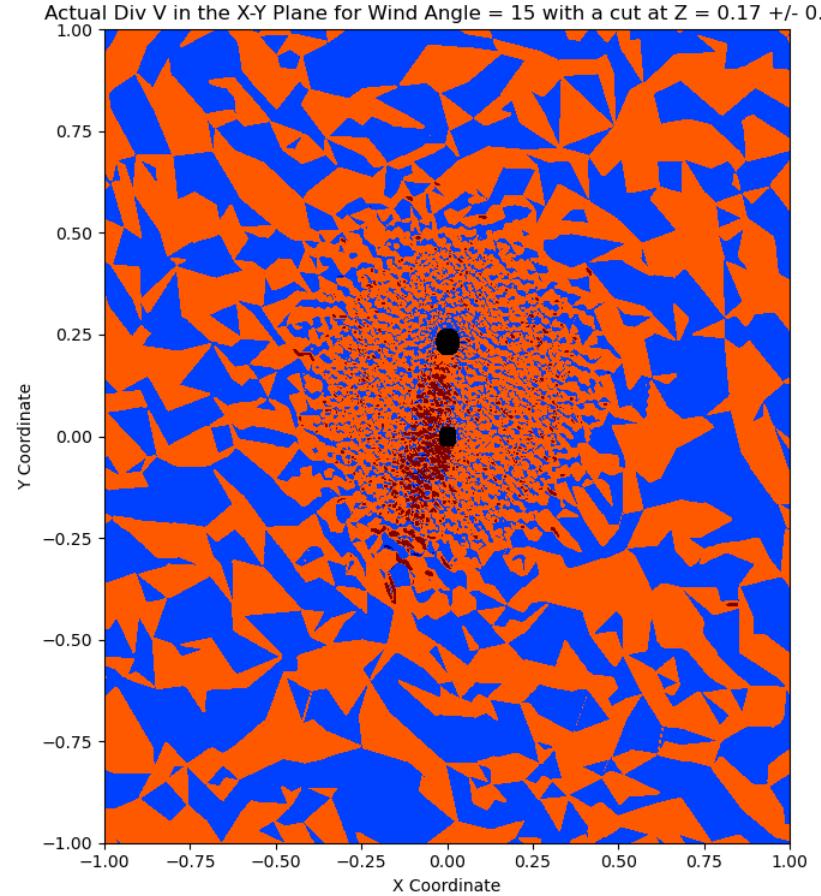
Comparison of Actual vs. Predicted values with Wind Angle = 0 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



Comparison of Actual vs. Predicted values with Wind Angle = 0 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02

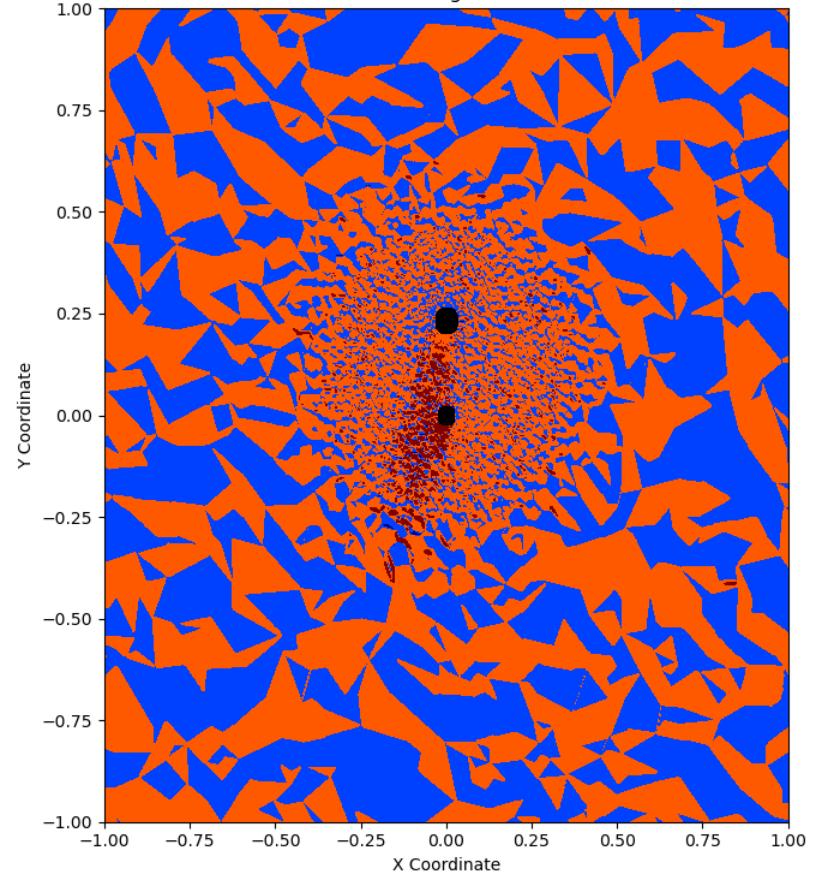


Comparison of Actual vs. Predicted values with Wind Angle = 15 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02

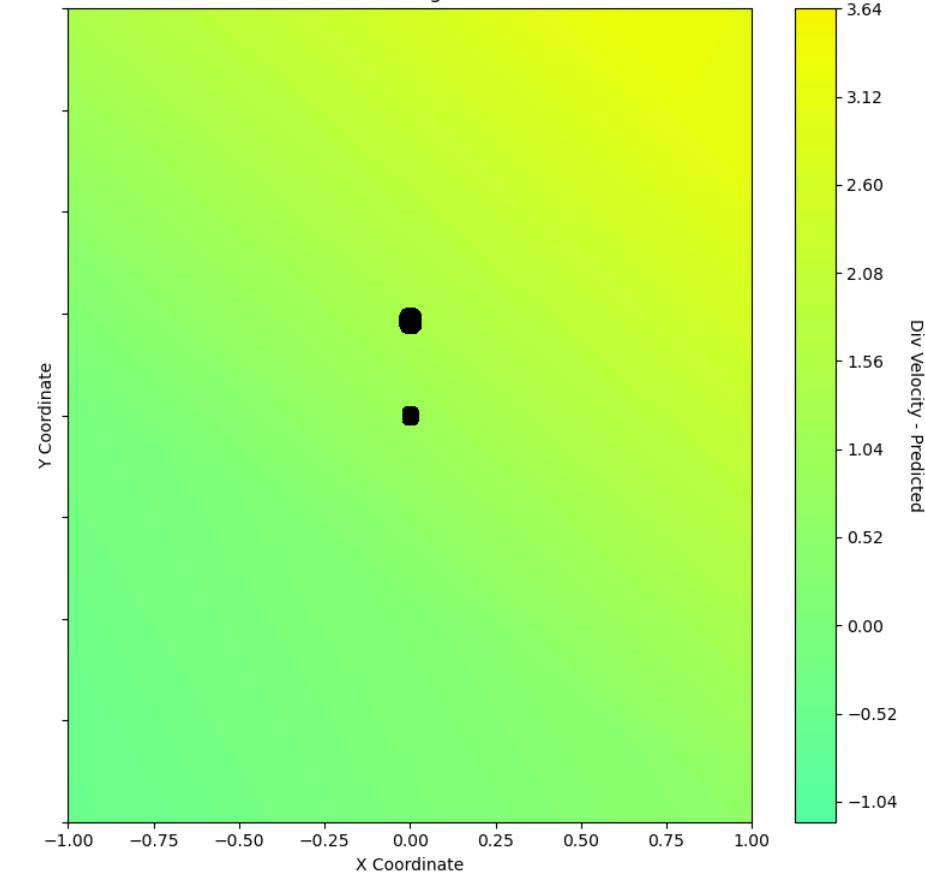


Comparison of Actual vs. Predicted values with Wind Angle = 15 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02

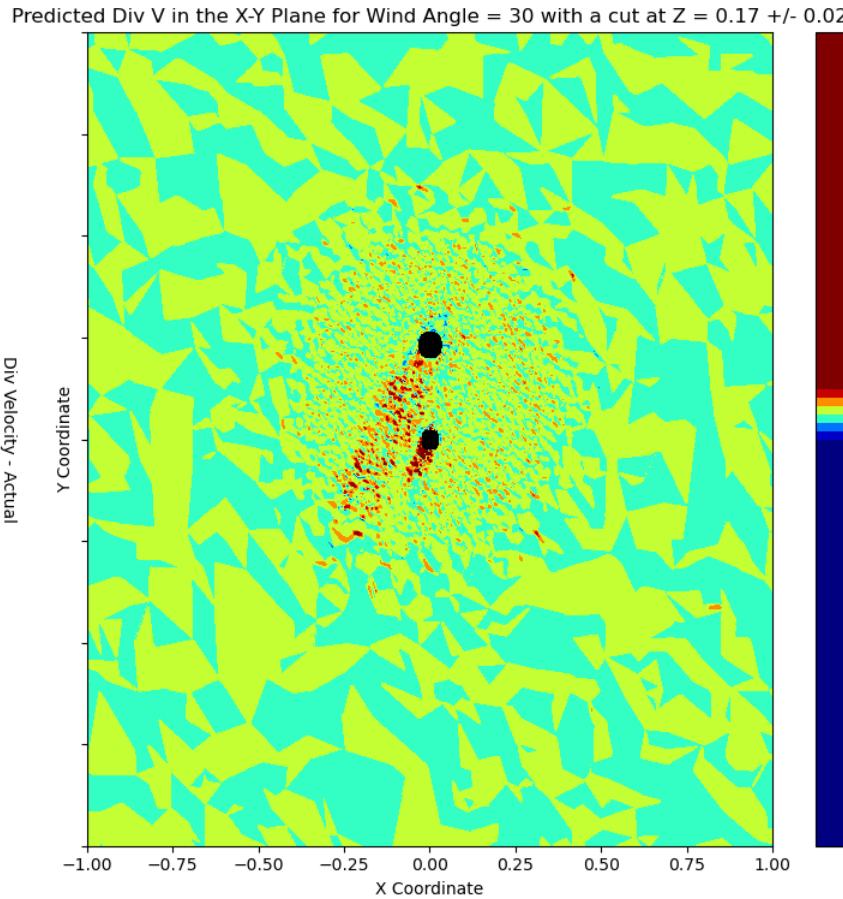
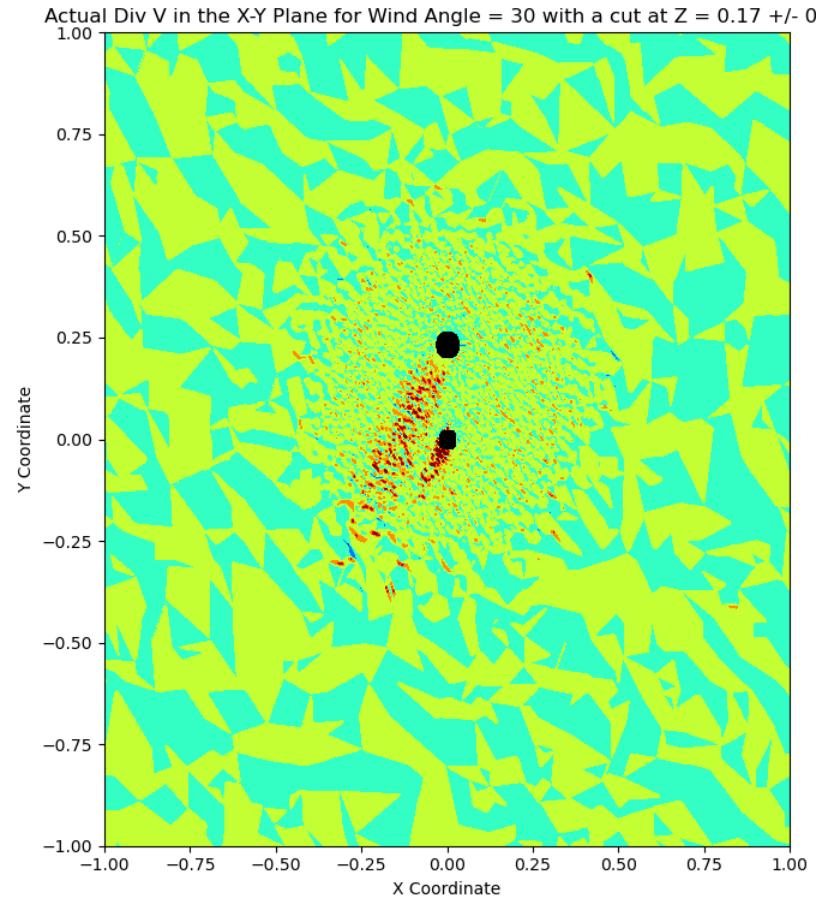
Actual Div V in the X-Y Plane for Wind Angle = 15 with a cut at Z = 0.17 +/- 0.02



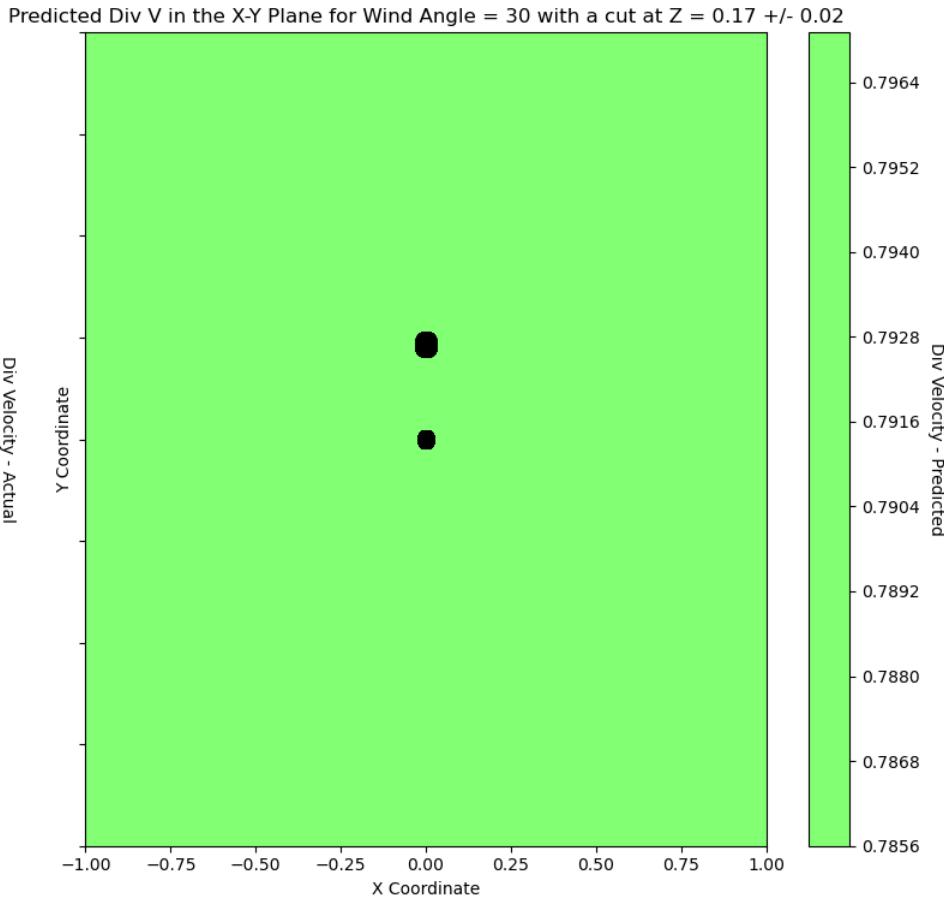
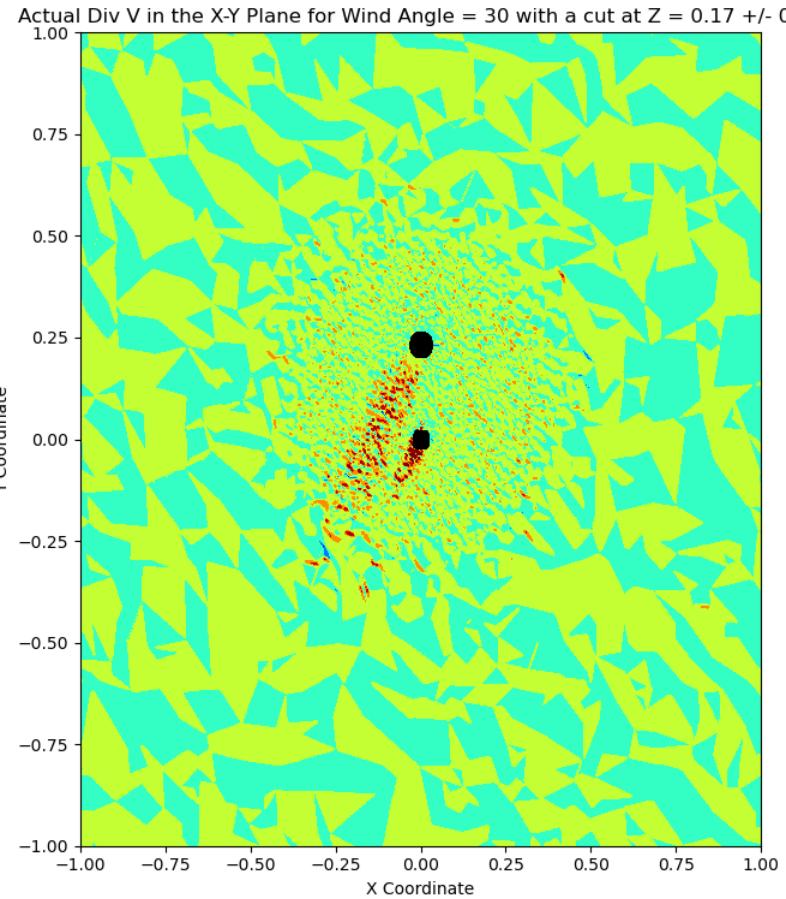
Predicted Div V in the X-Y Plane for Wind Angle = 15 with a cut at Z = 0.17 +/- 0.02



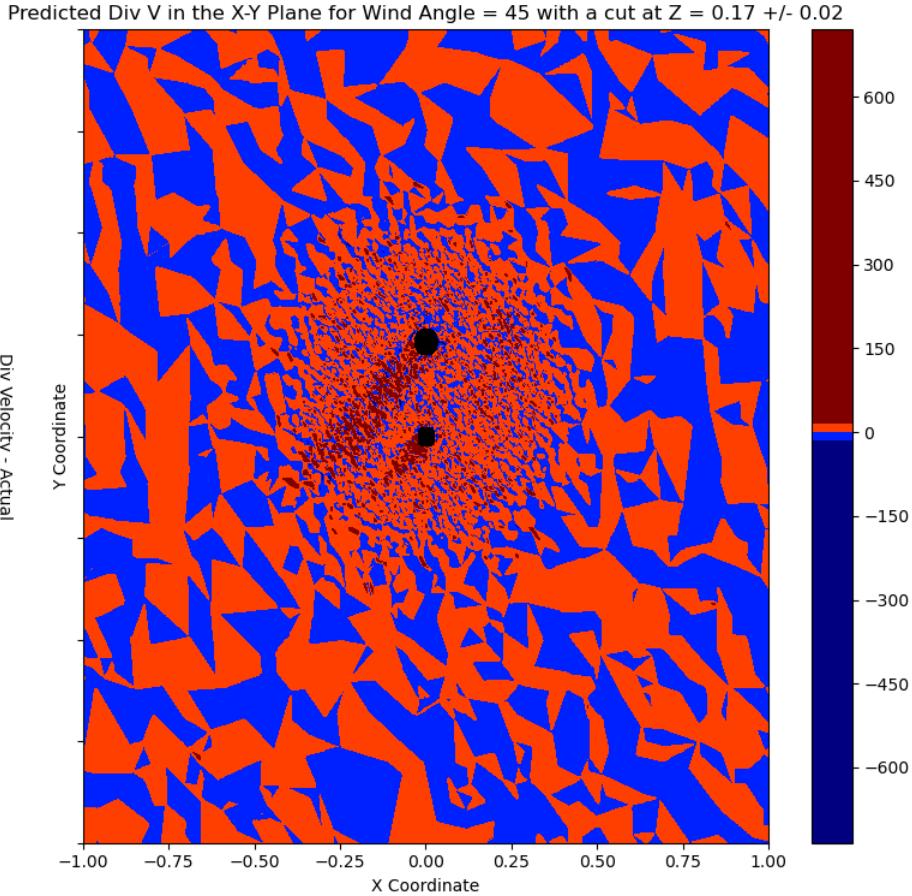
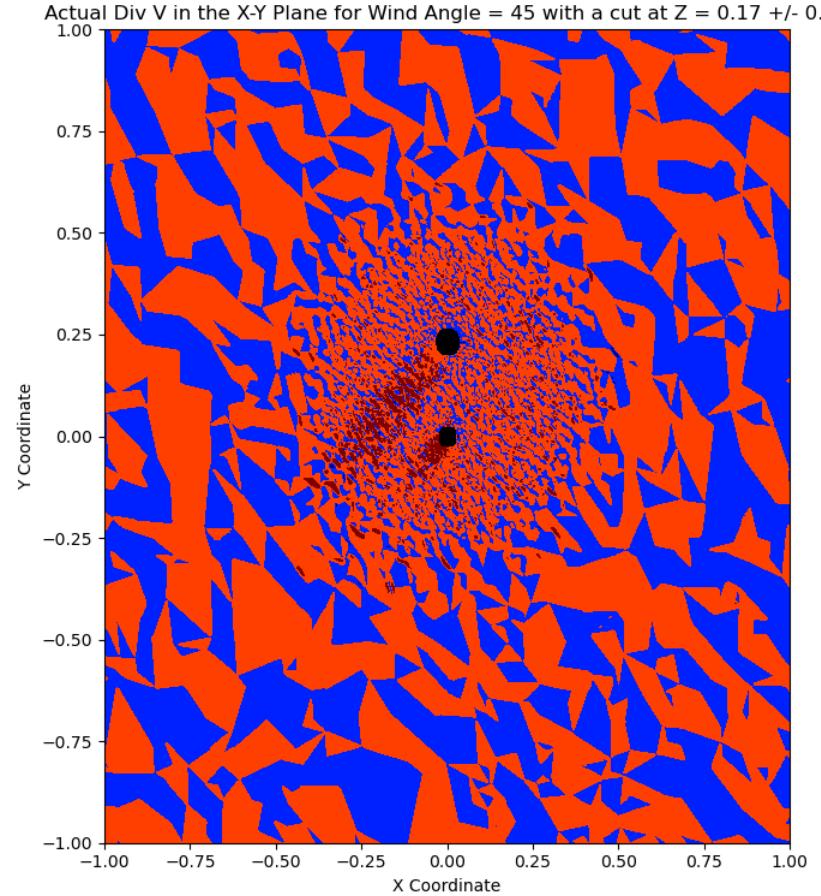
Comparison of Actual vs. Predicted values with Wind Angle = 30 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



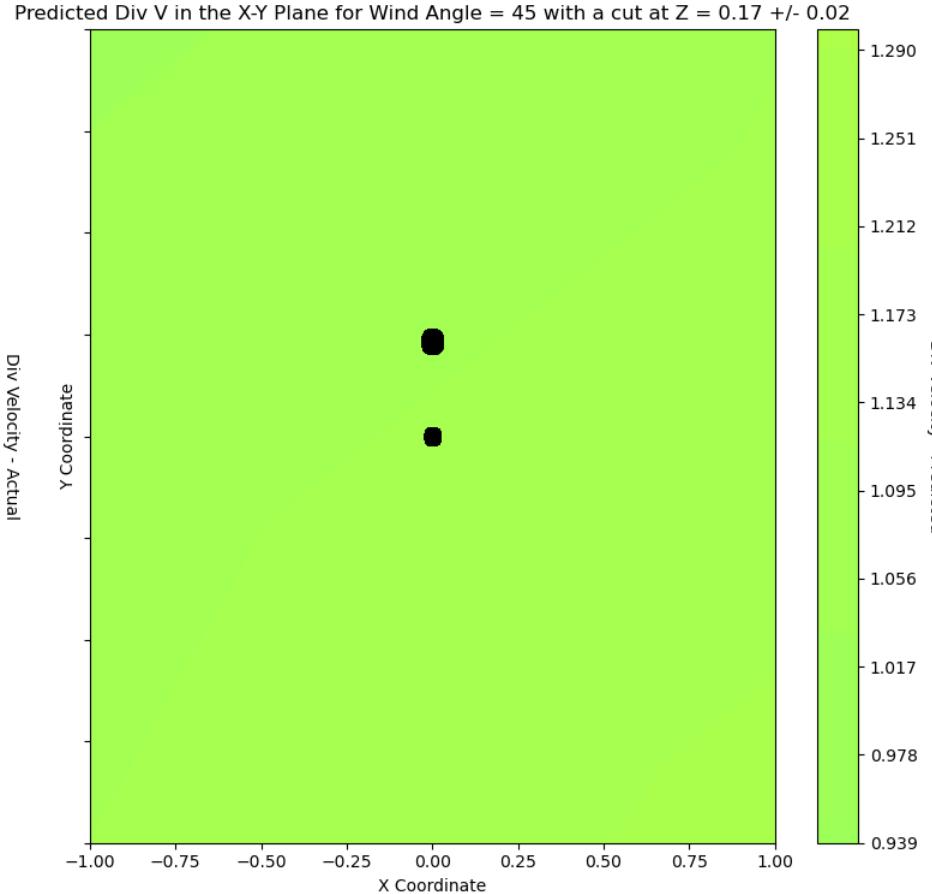
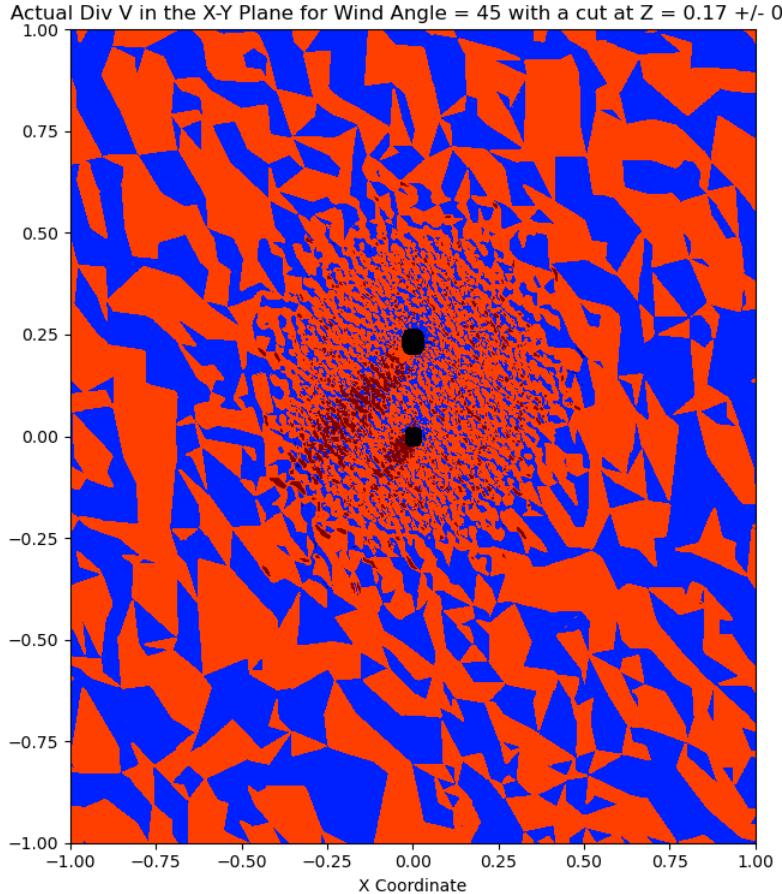
Comparison of Actual vs. Predicted values with Wind Angle = 30 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



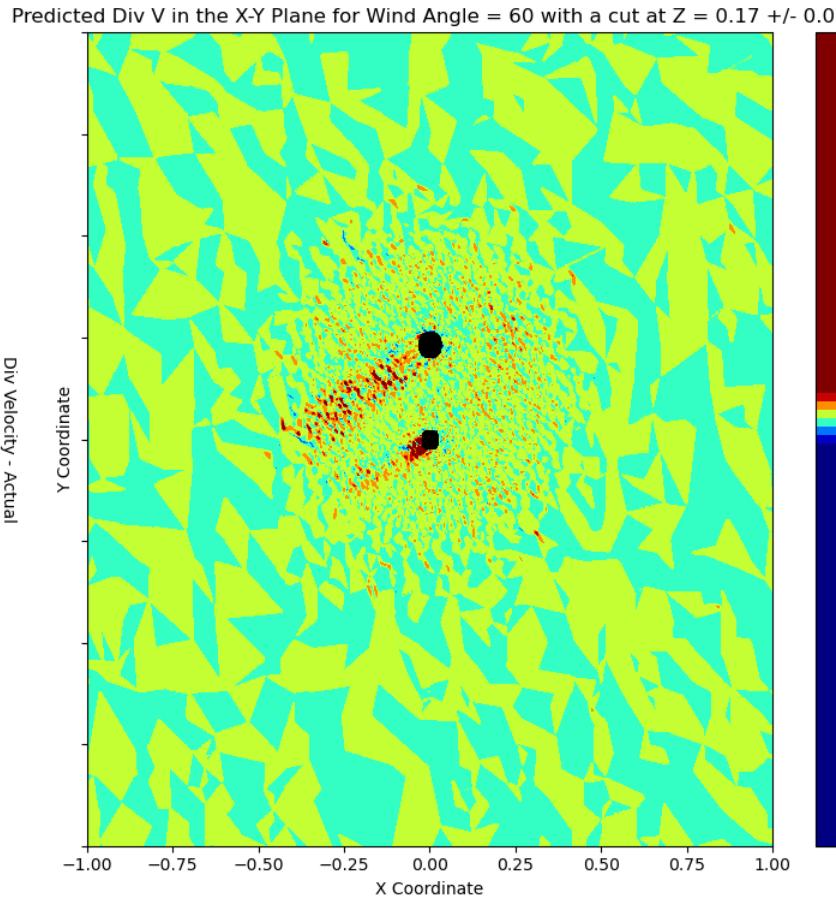
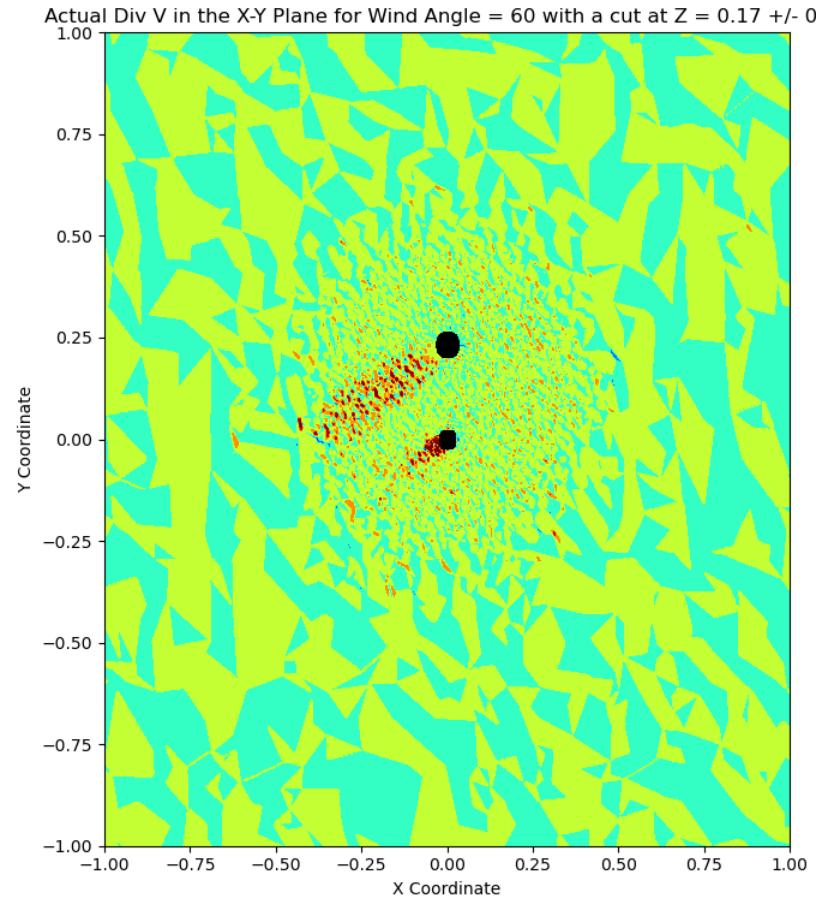
Comparison of Actual vs. Predicted values with Wind Angle = 45 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



Comparison of Actual vs. Predicted values with Wind Angle = 45 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02

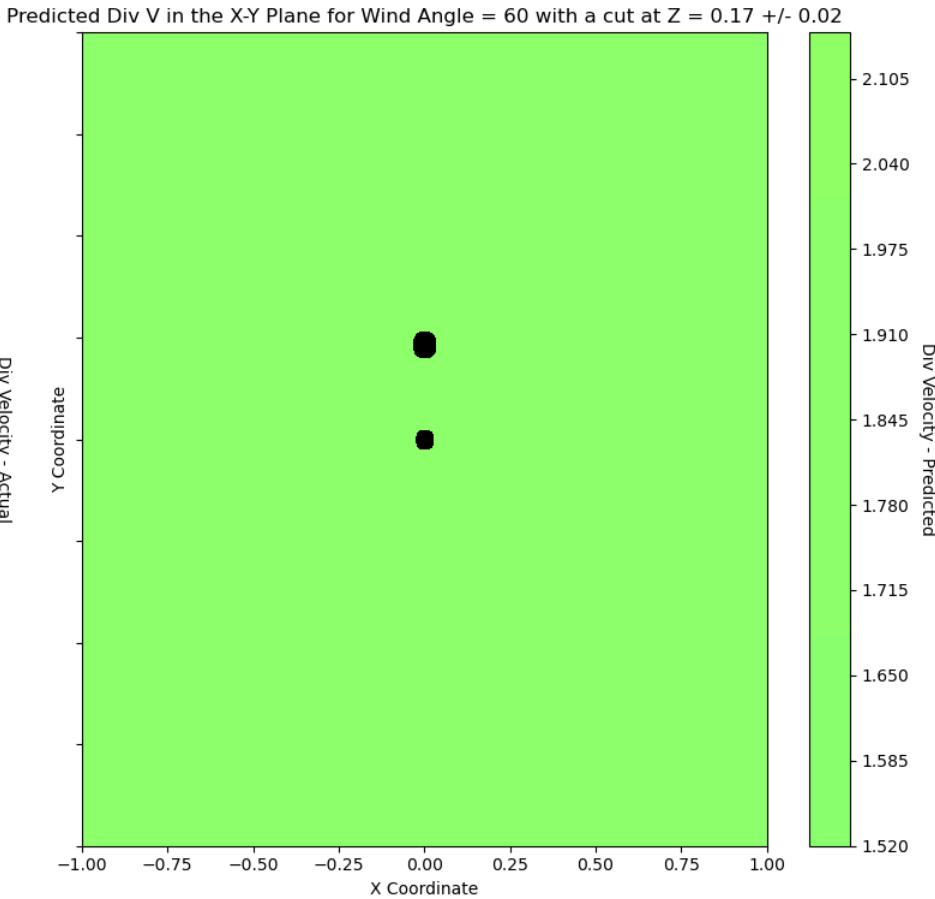
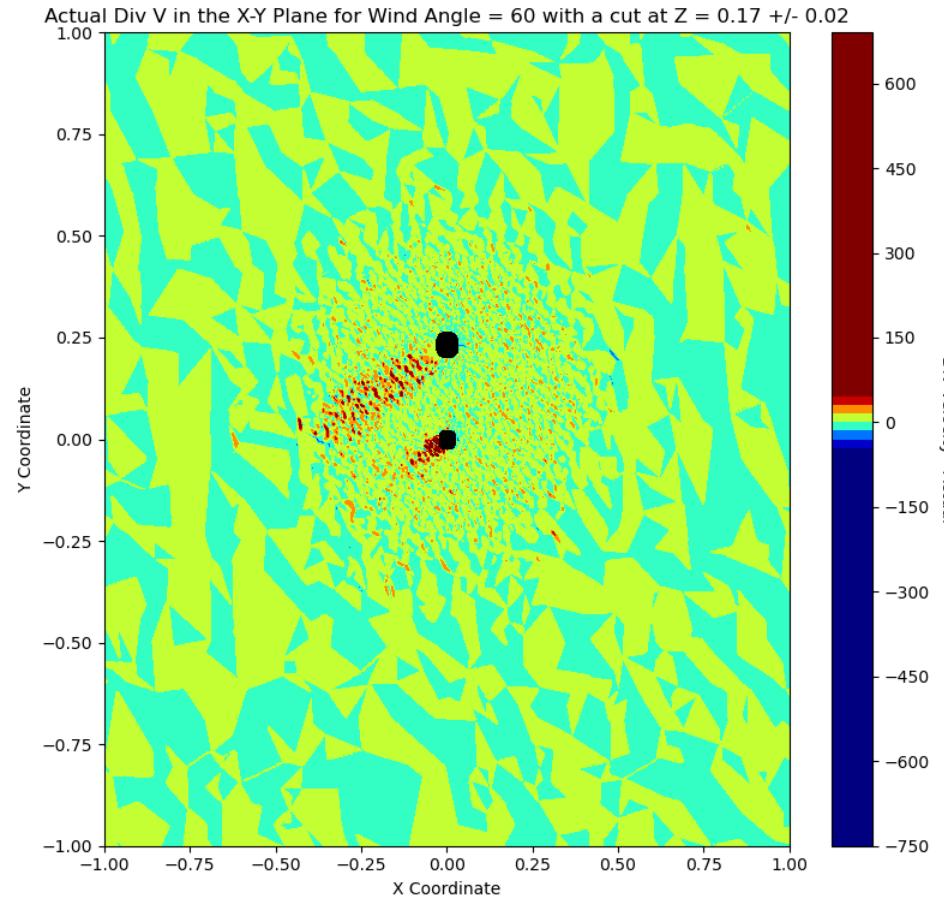


Comparison of Actual vs. Predicted values with Wind Angle = 60 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02

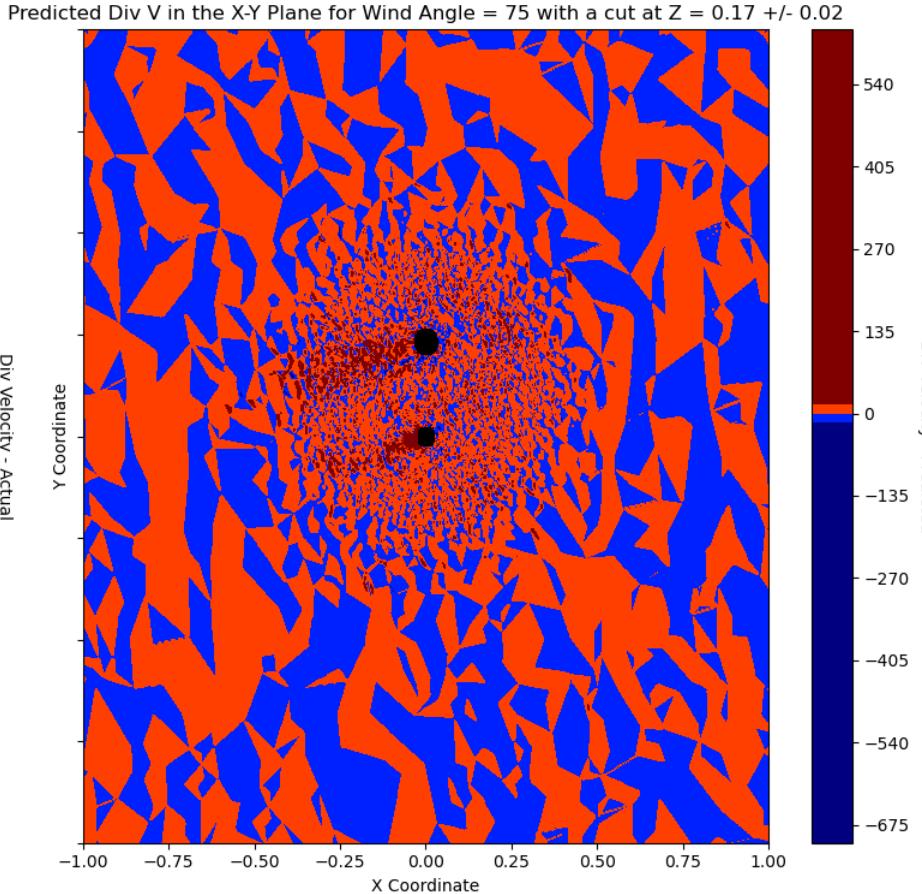
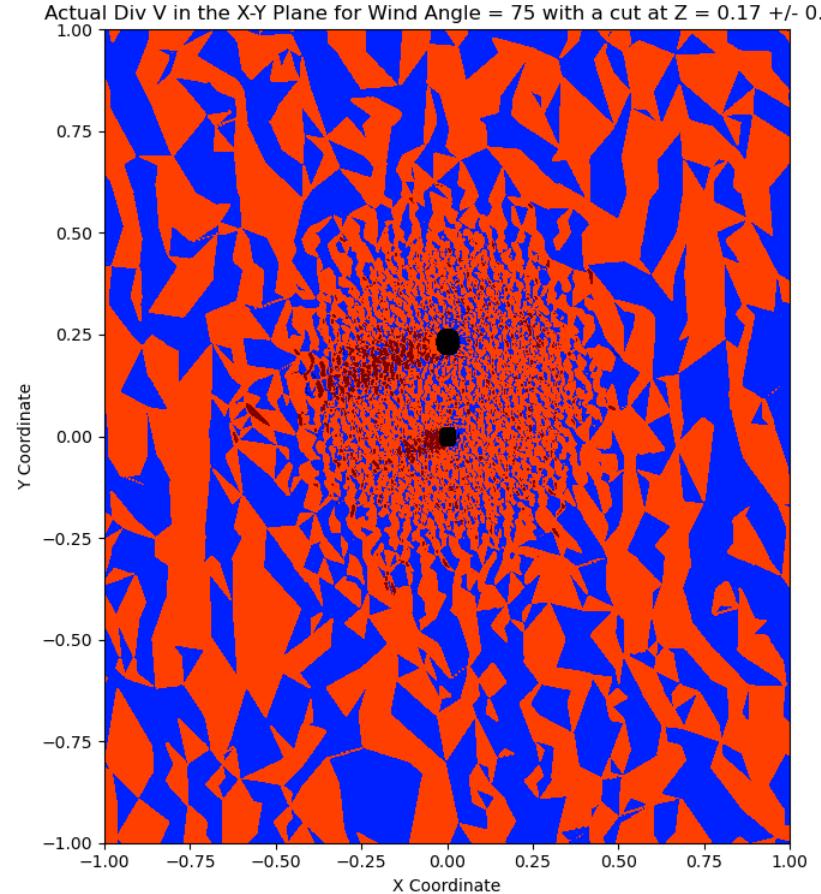


Div Velocity - Predicted

Comparison of Actual vs. Predicted values with Wind Angle = 60 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02

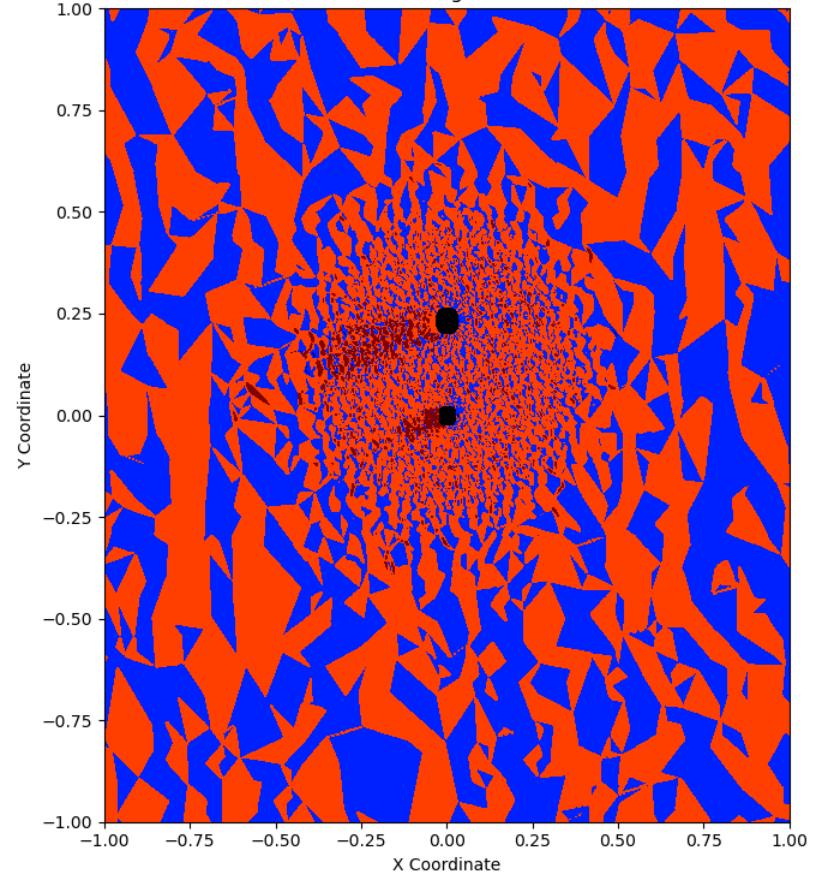


Comparison of Actual vs. Predicted values with Wind Angle = 75 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02

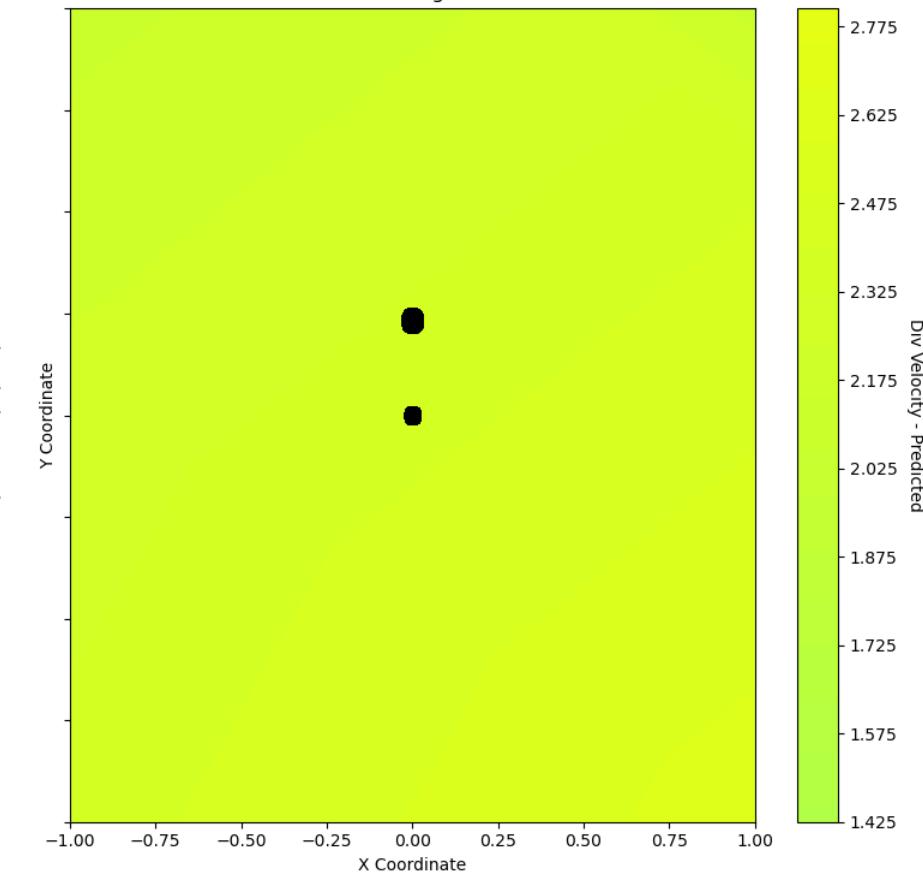


Comparison of Actual vs. Predicted values with Wind Angle = 75 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02

Actual Div V in the X-Y Plane for Wind Angle = 75 with a cut at Z = 0.17 +/- 0.02

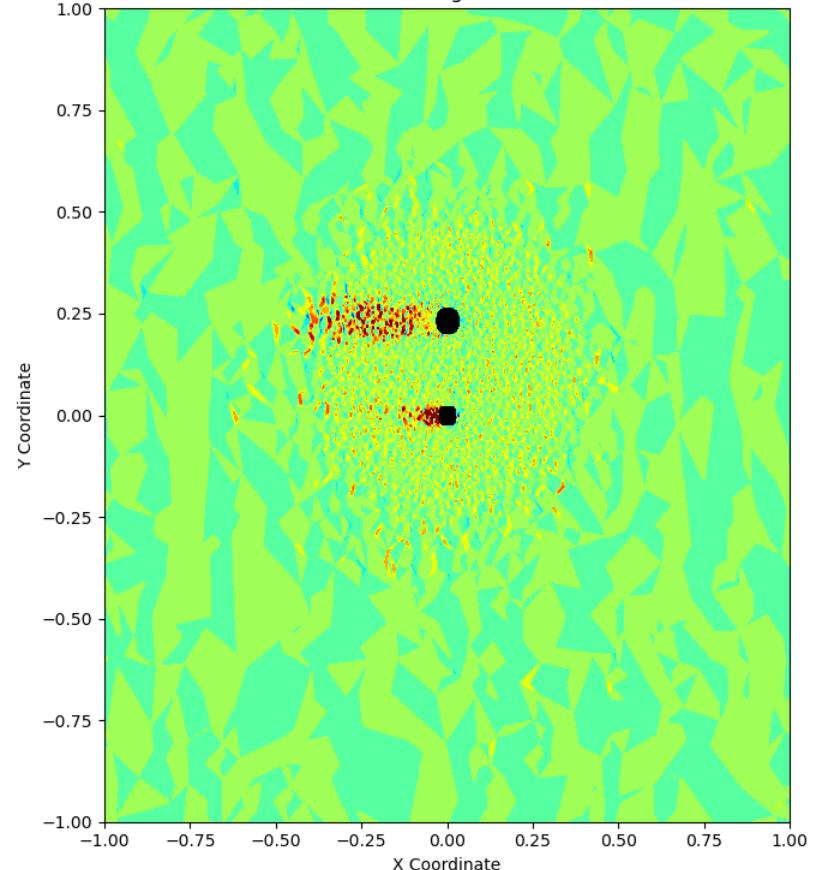


Predicted Div V in the X-Y Plane for Wind Angle = 75 with a cut at Z = 0.17 +/- 0.02

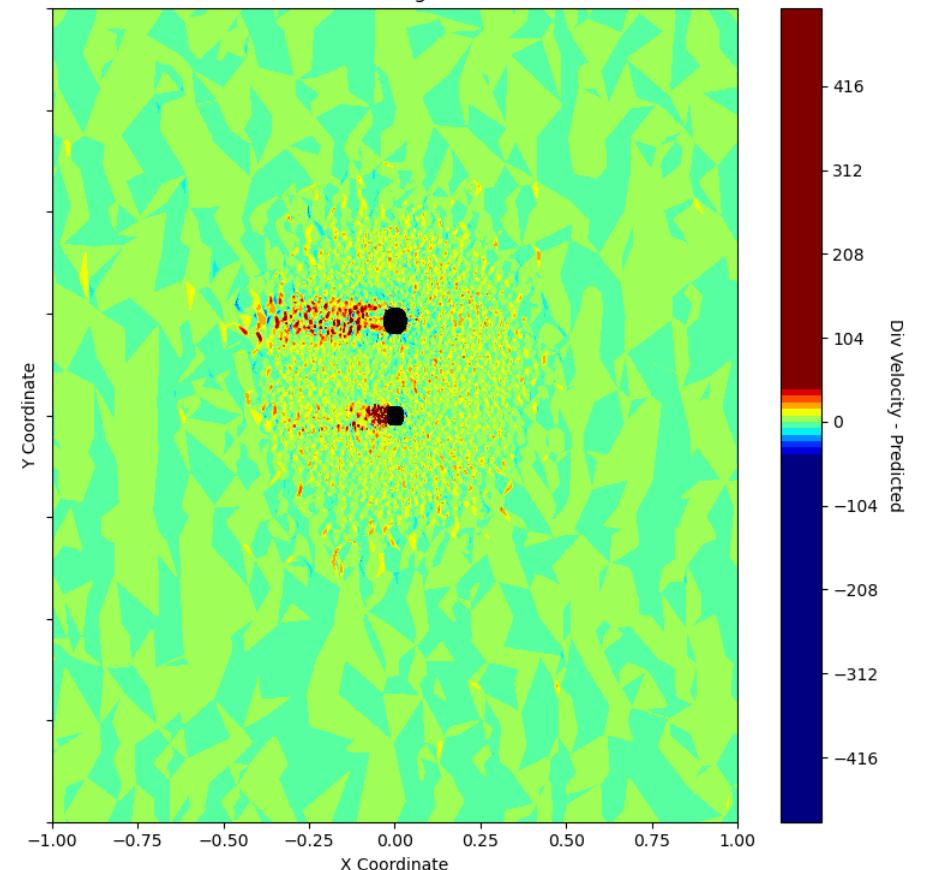


Comparison of Actual vs. Predicted values with Wind Angle = 90 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02

Actual Div V in the X-Y Plane for Wind Angle = 90 with a cut at Z = 0.17 +/- 0.02

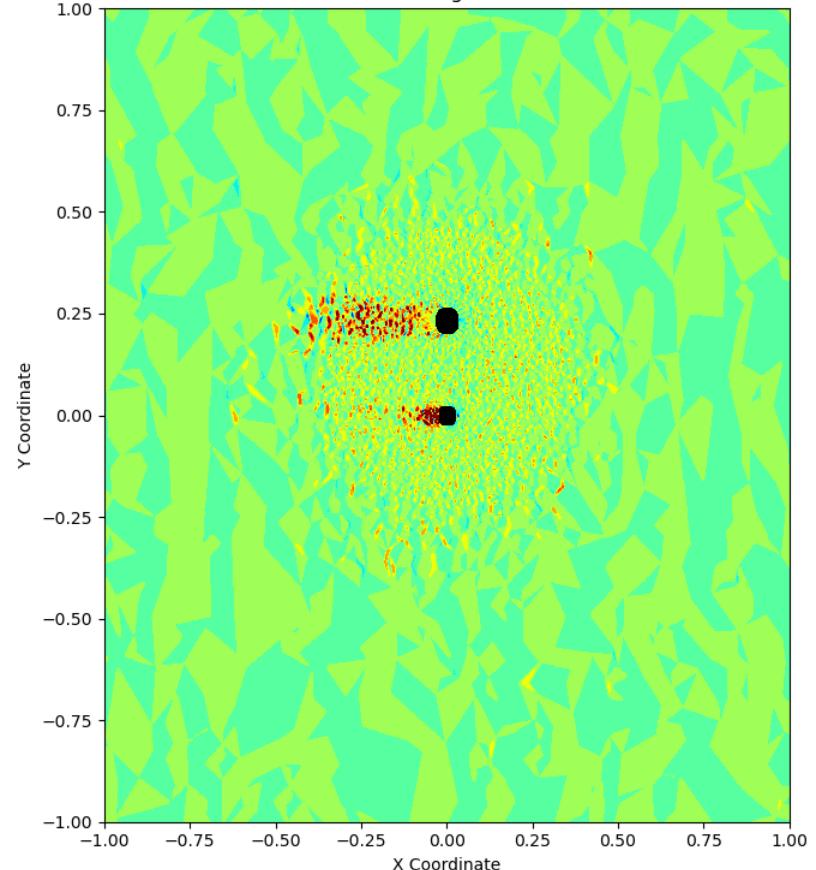


Predicted Div V in the X-Y Plane for Wind Angle = 90 with a cut at Z = 0.17 +/- 0.02

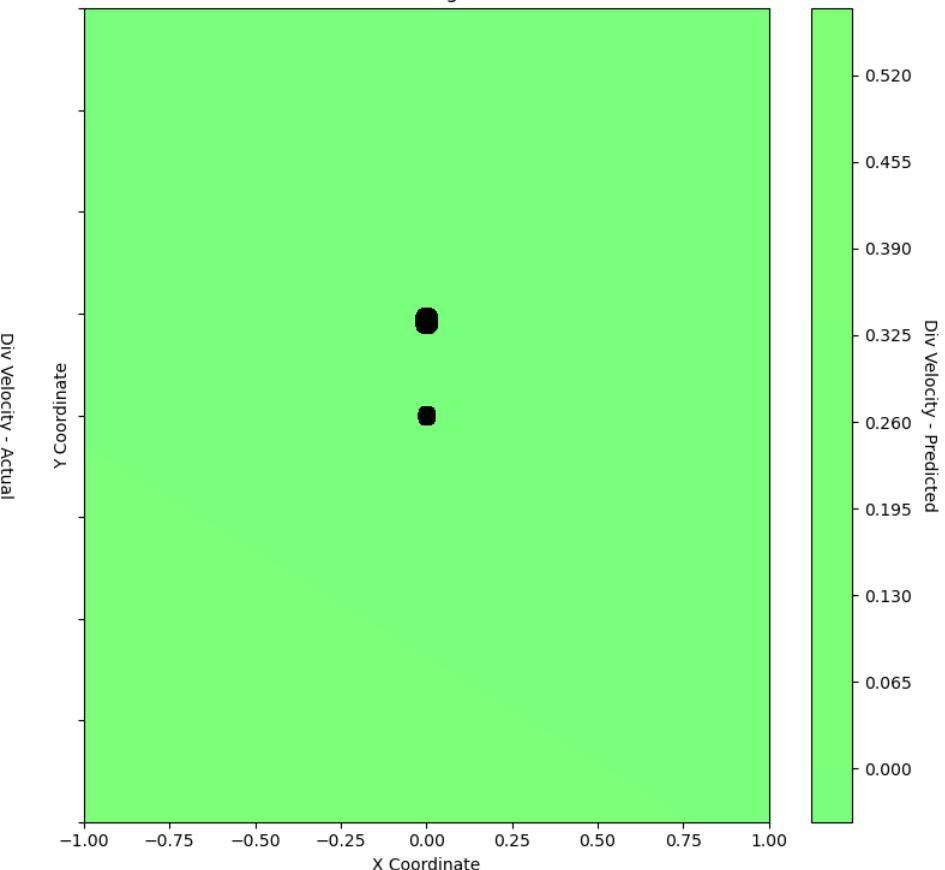


Comparison of Actual vs. Predicted values with Wind Angle = 90 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02

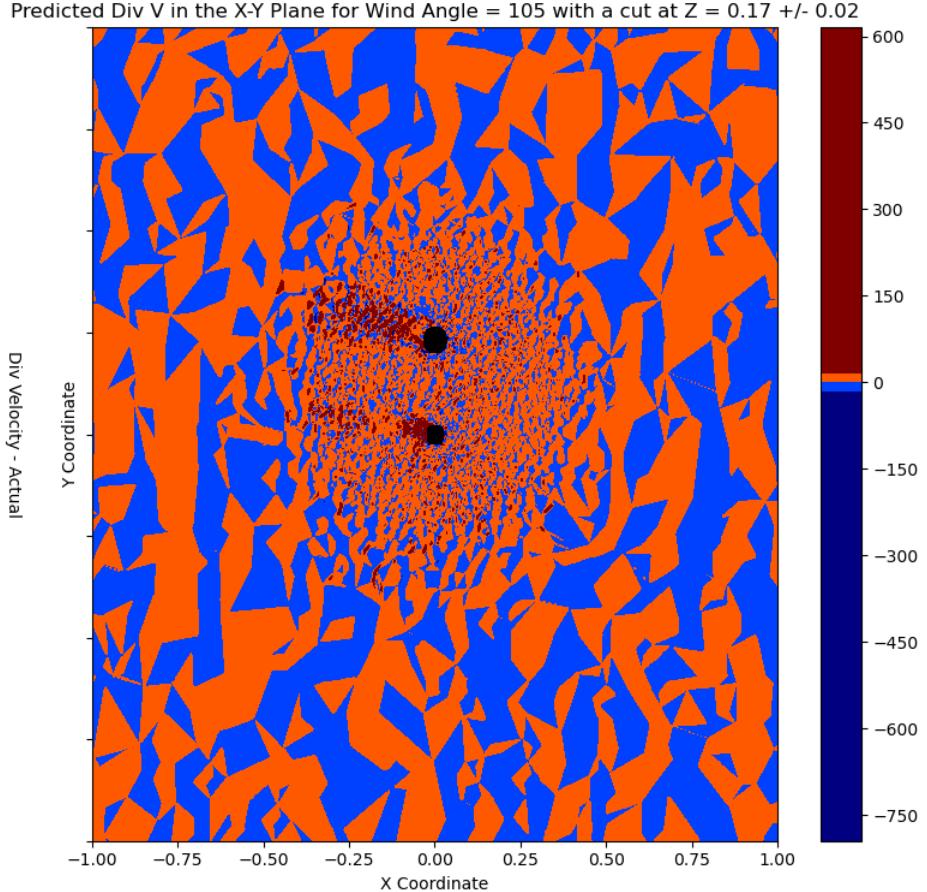
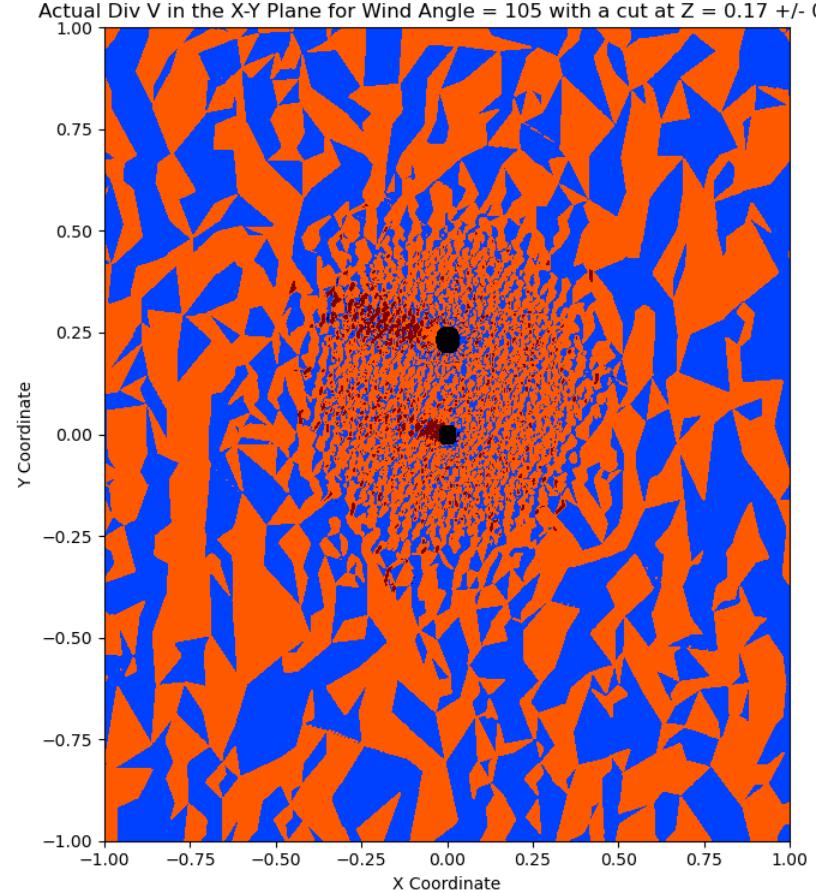
Actual Div V in the X-Y Plane for Wind Angle = 90 with a cut at Z = 0.17 +/- 0.02



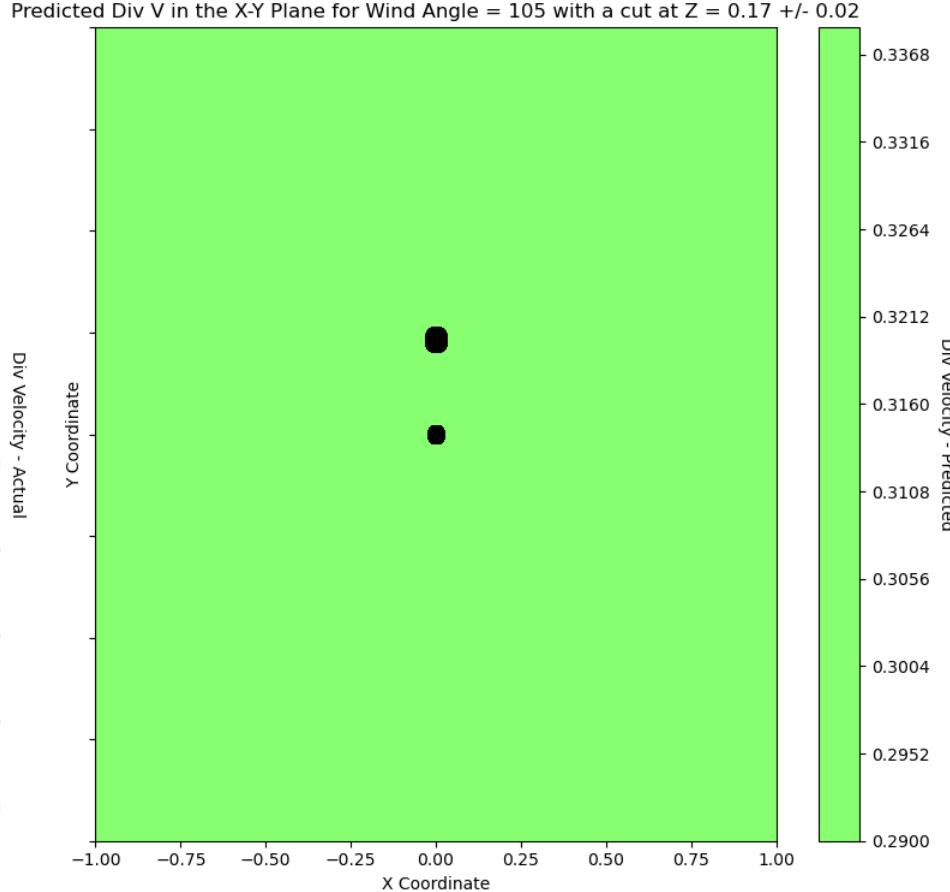
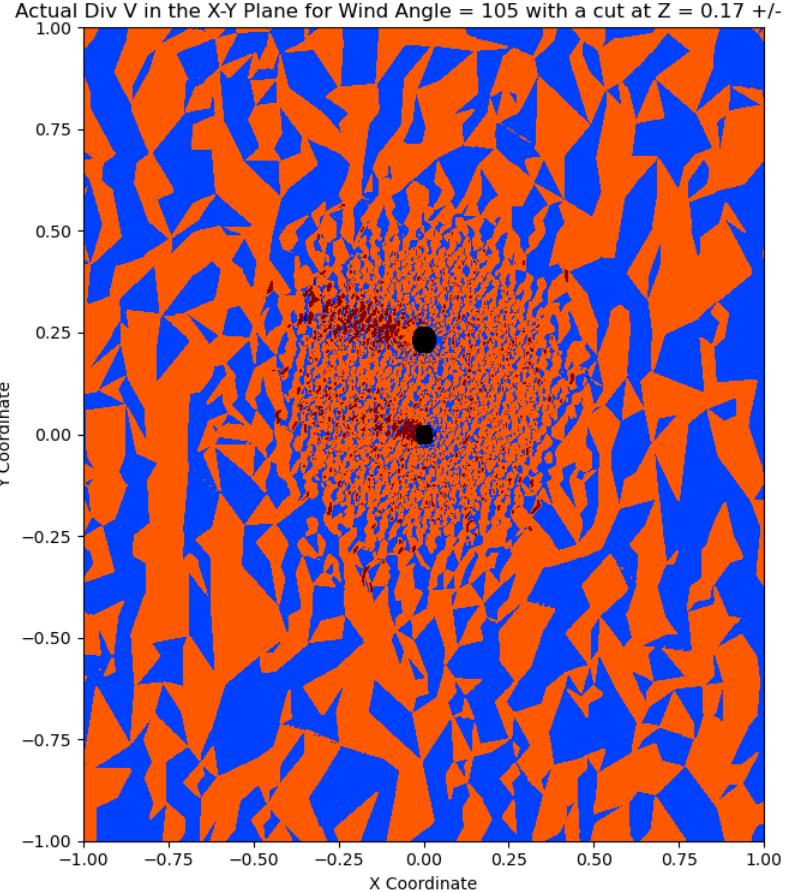
Predicted Div V in the X-Y Plane for Wind Angle = 90 with a cut at Z = 0.17 +/- 0.02



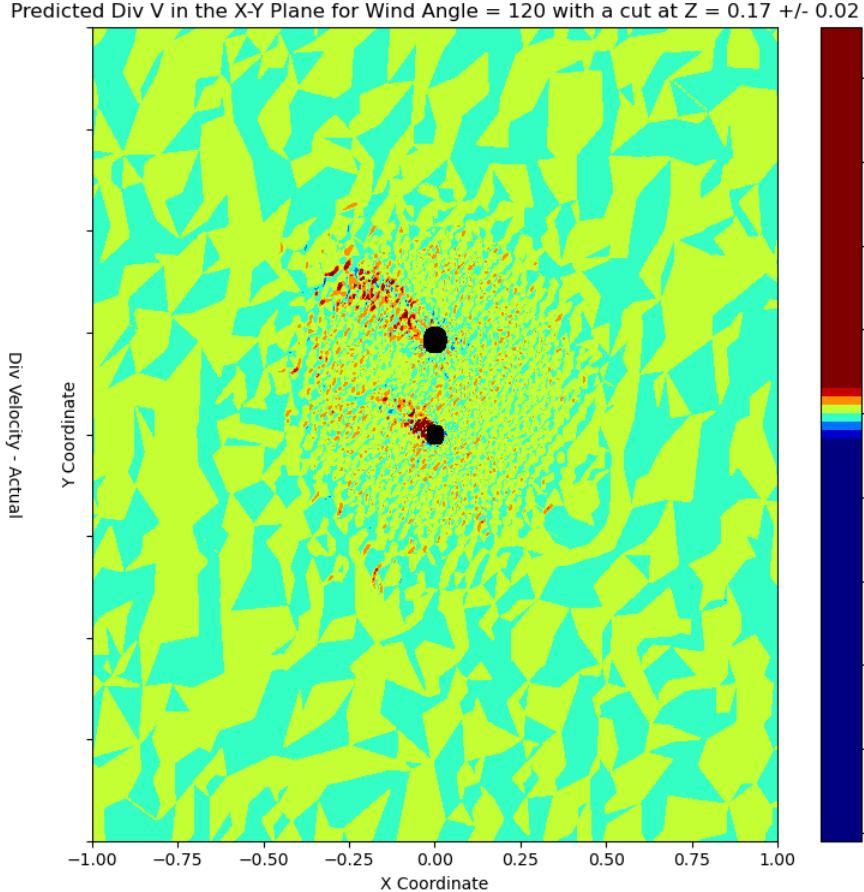
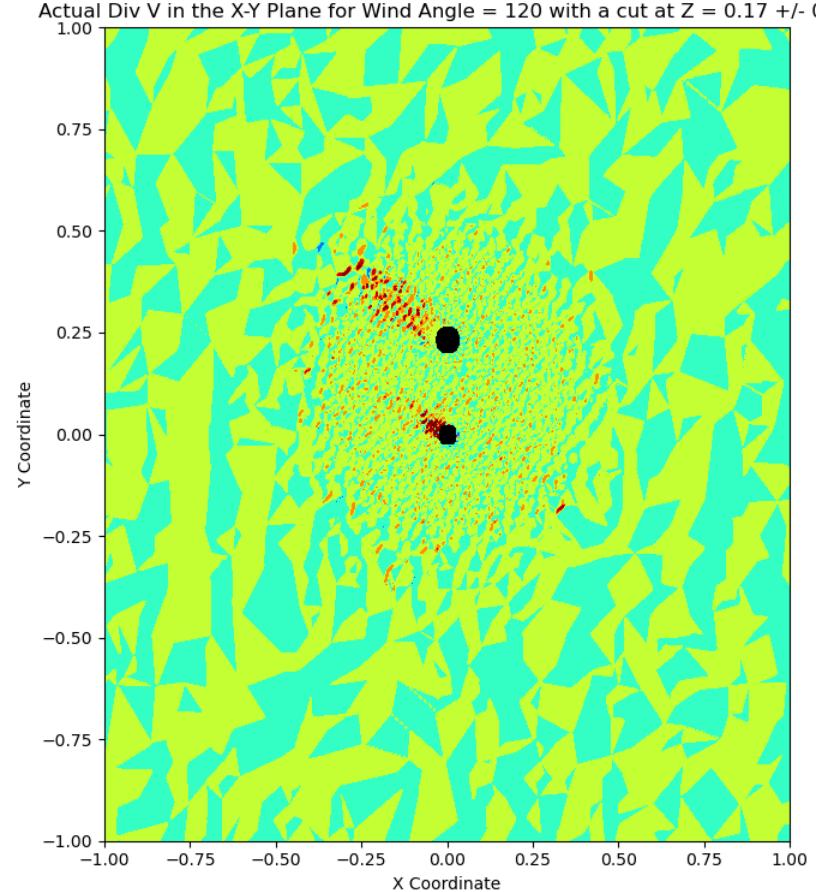
Comparison of Actual vs. Predicted values with Wind Angle = 105 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



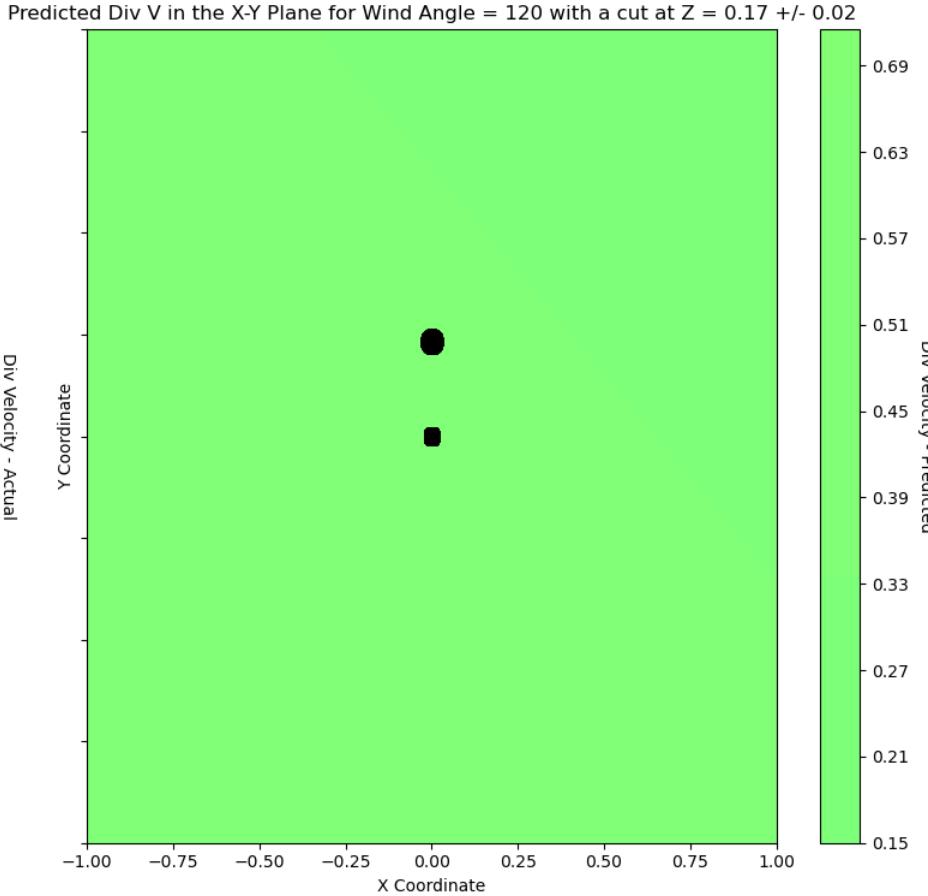
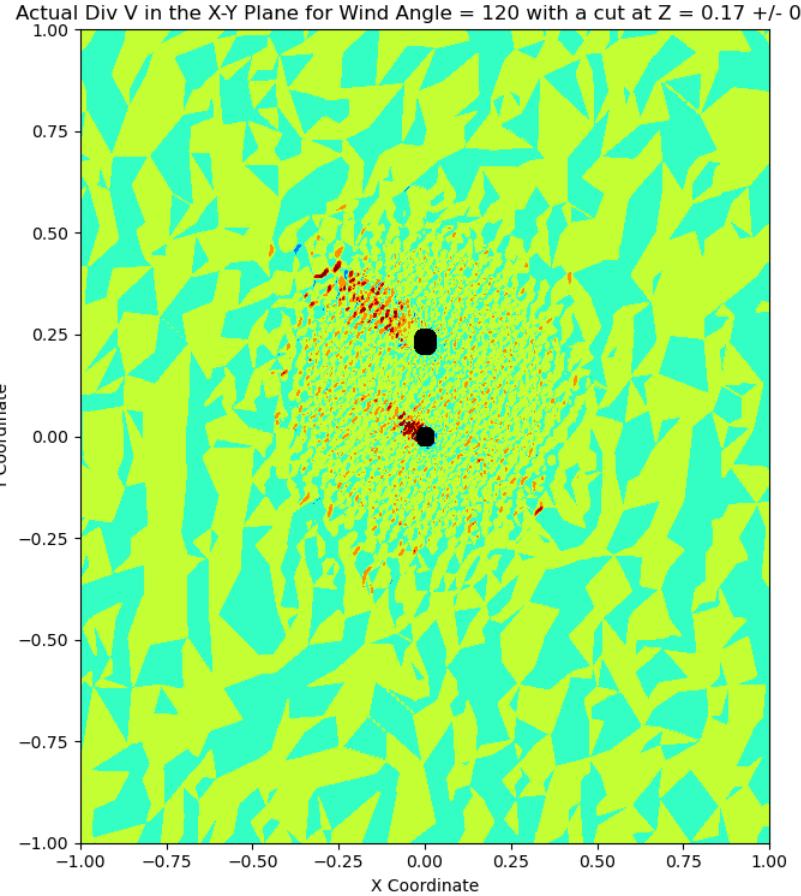
Comparison of Actual vs. Predicted values with Wind Angle = 105 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



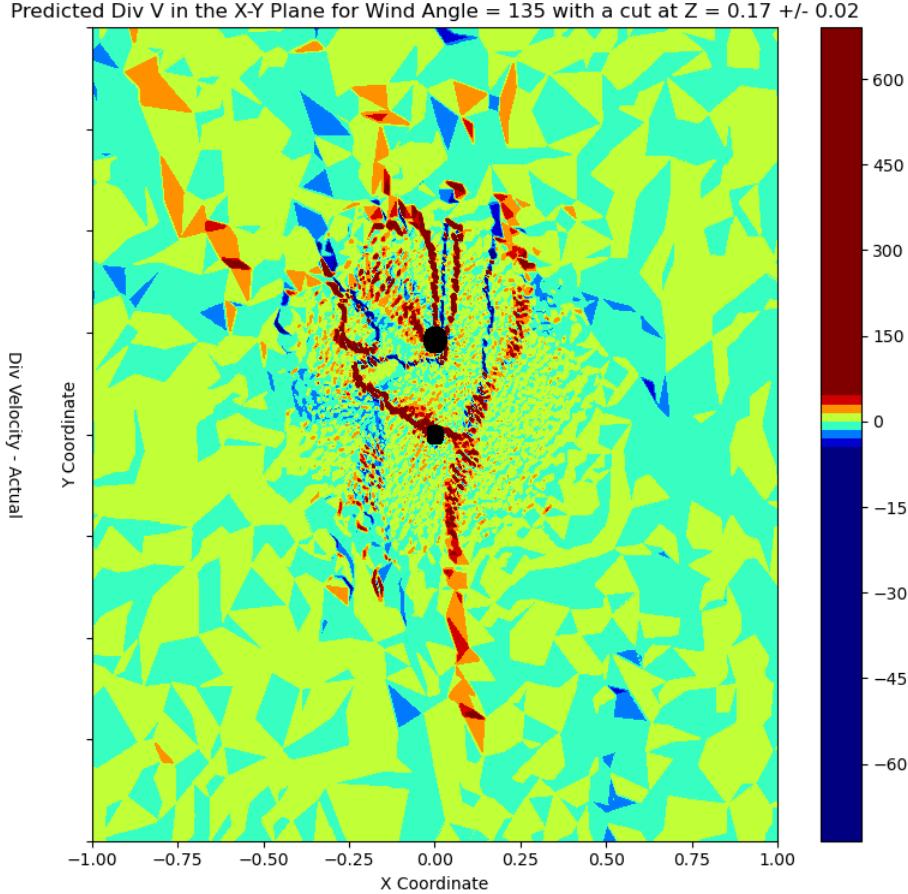
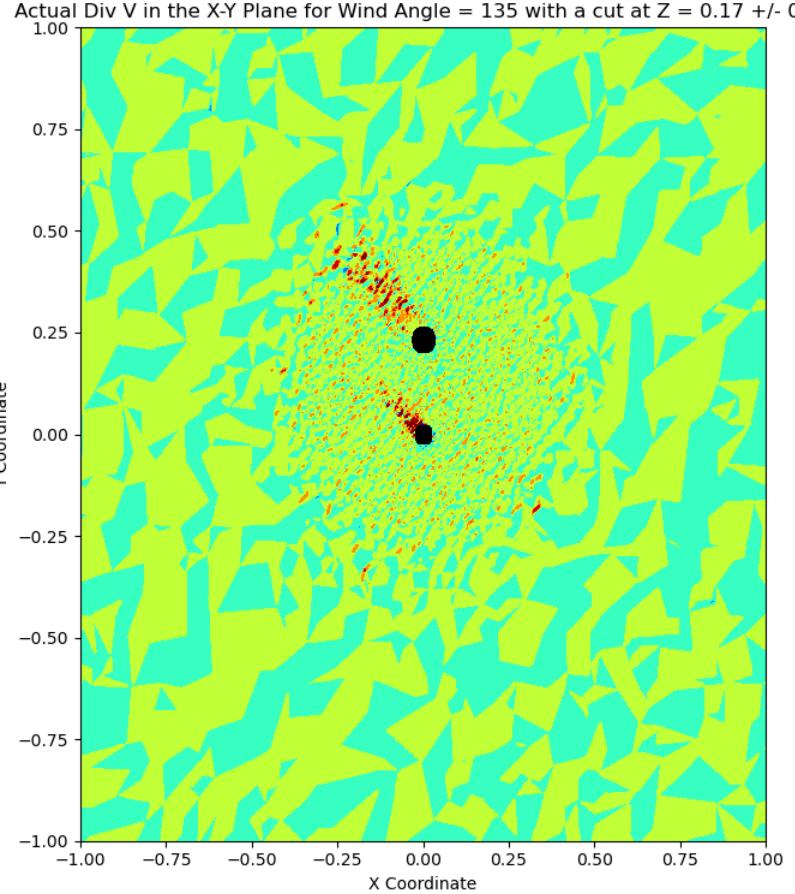
Comparison of Actual vs. Predicted values with Wind Angle = 120 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



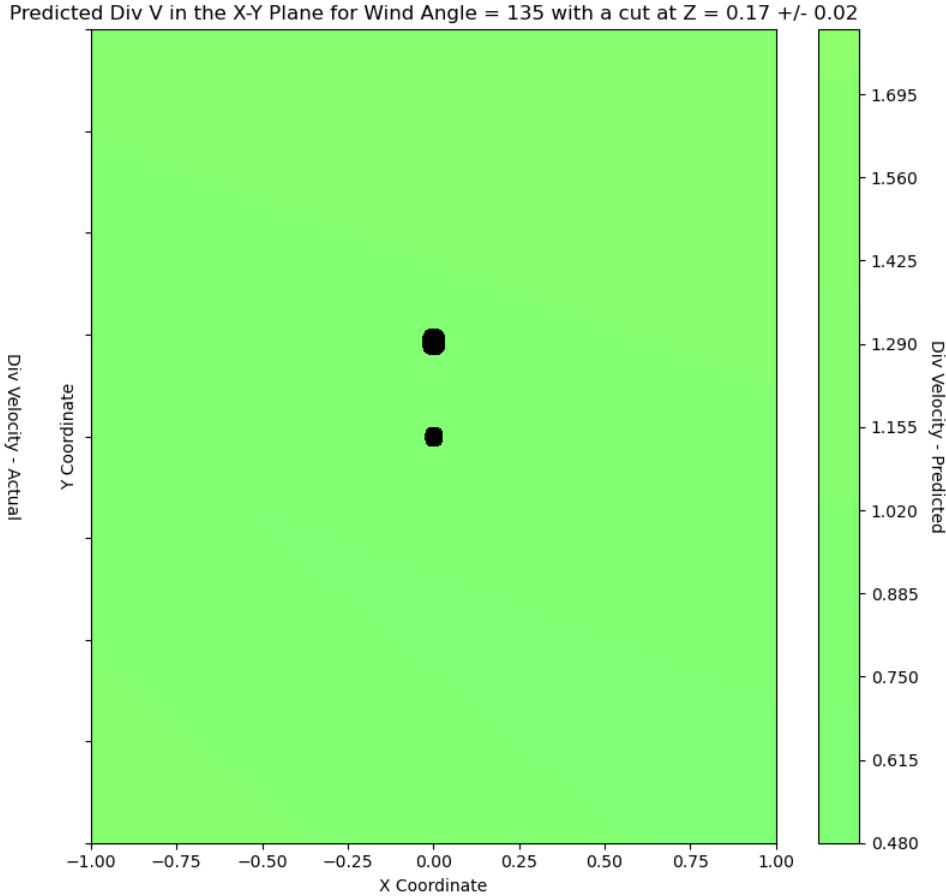
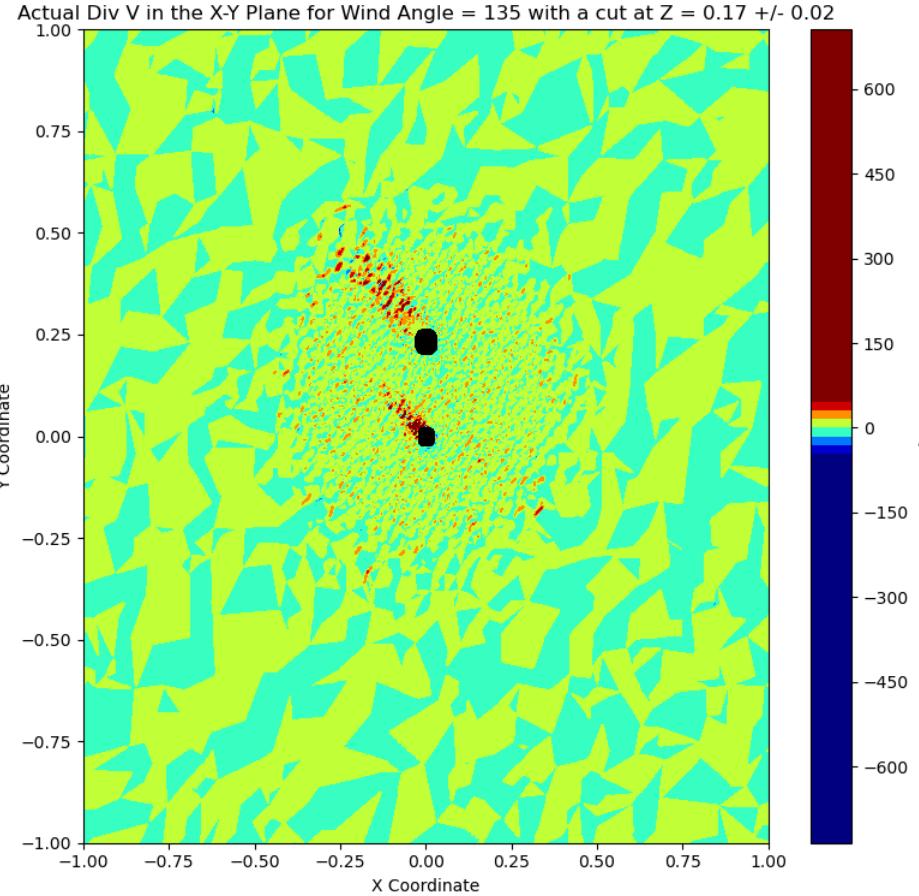
Comparison of Actual vs. Predicted values with Wind Angle = 120 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



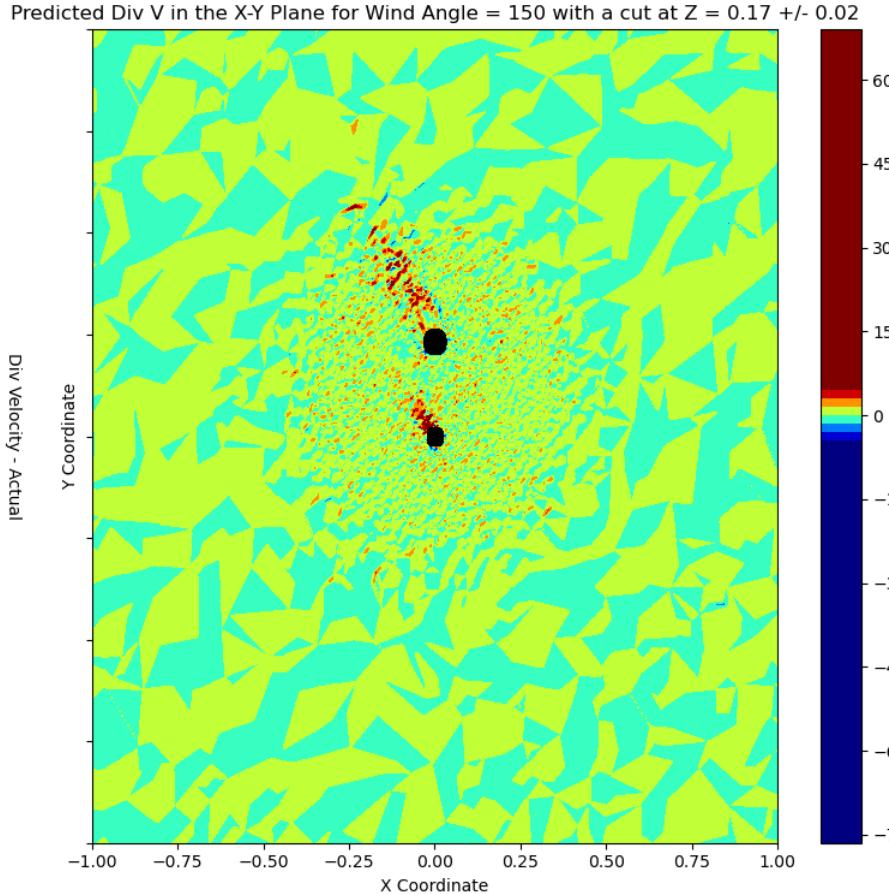
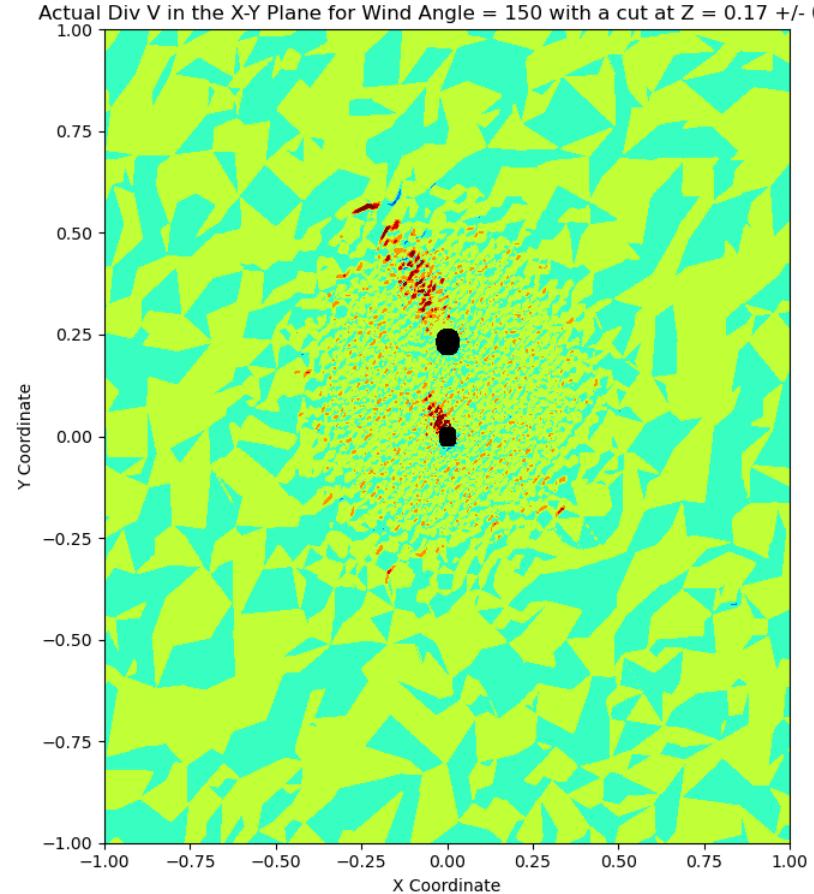
Comparison of Actual vs. Predicted values with Wind Angle = 135 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



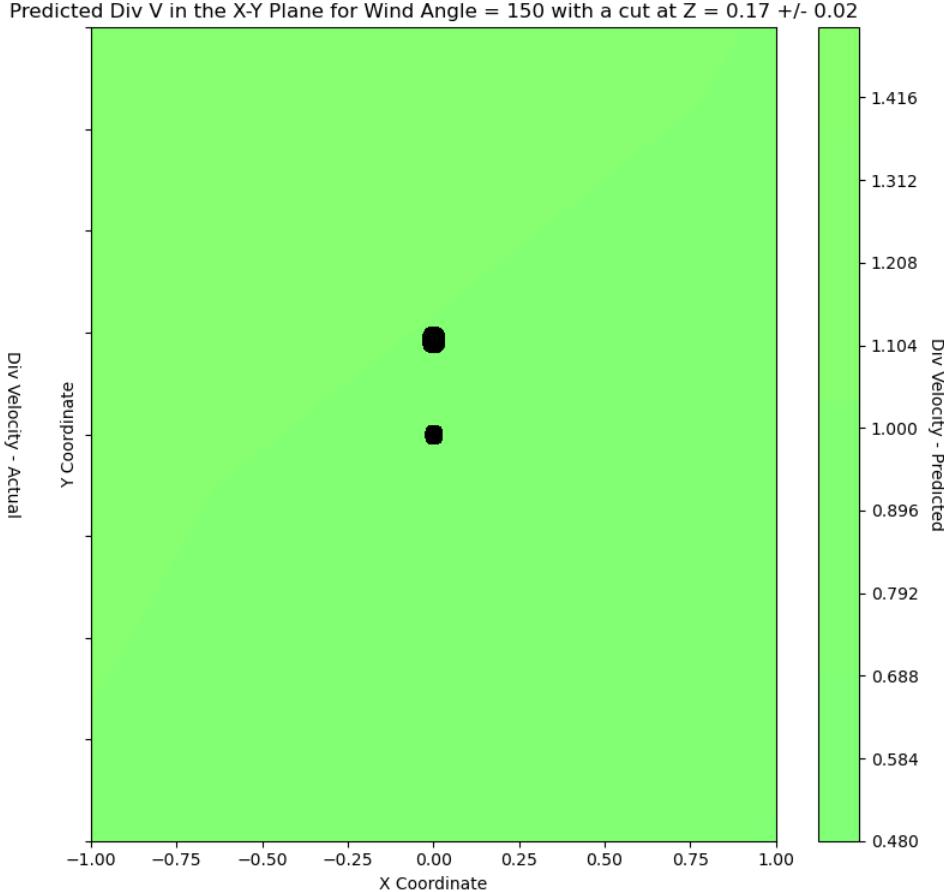
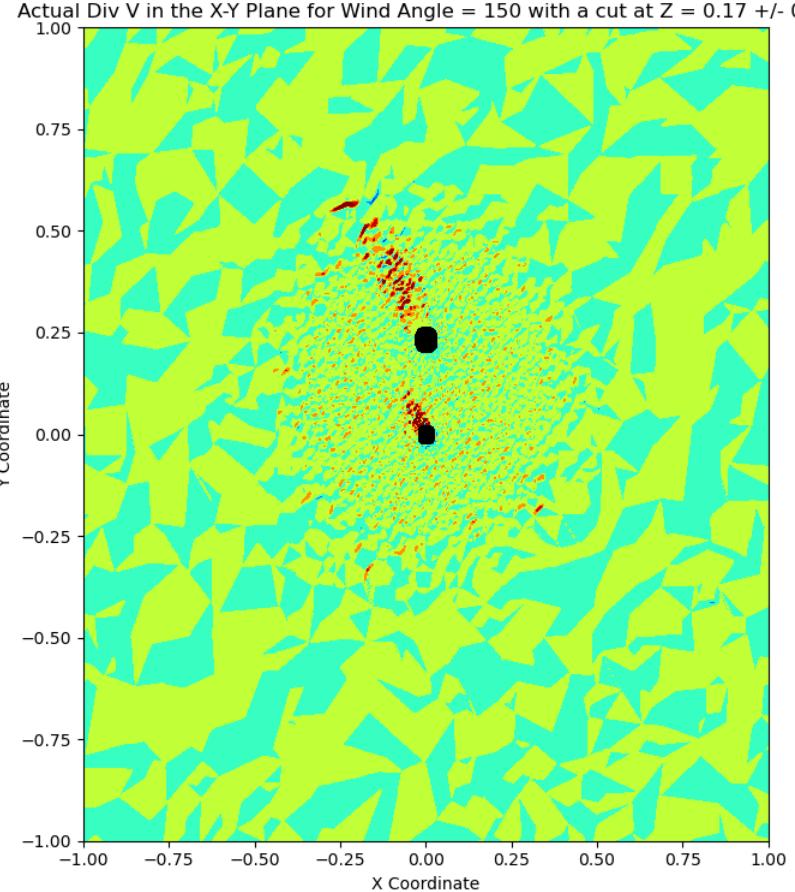
Comparison of Actual vs. Predicted values with Wind Angle = 135 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



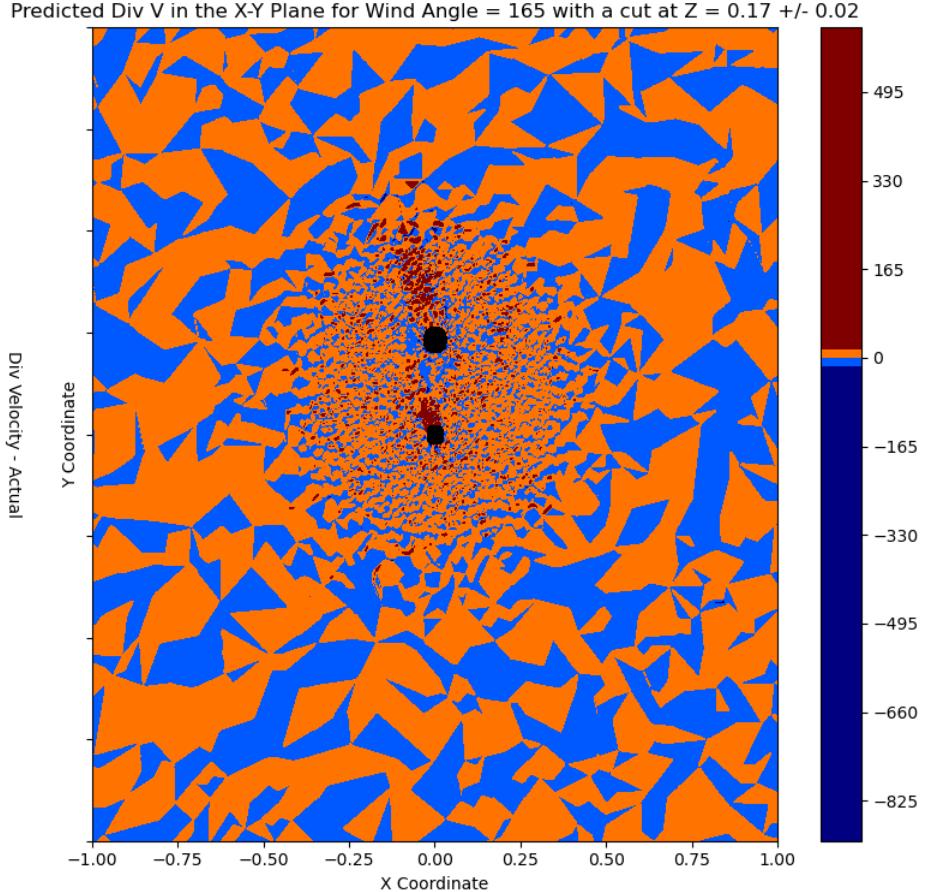
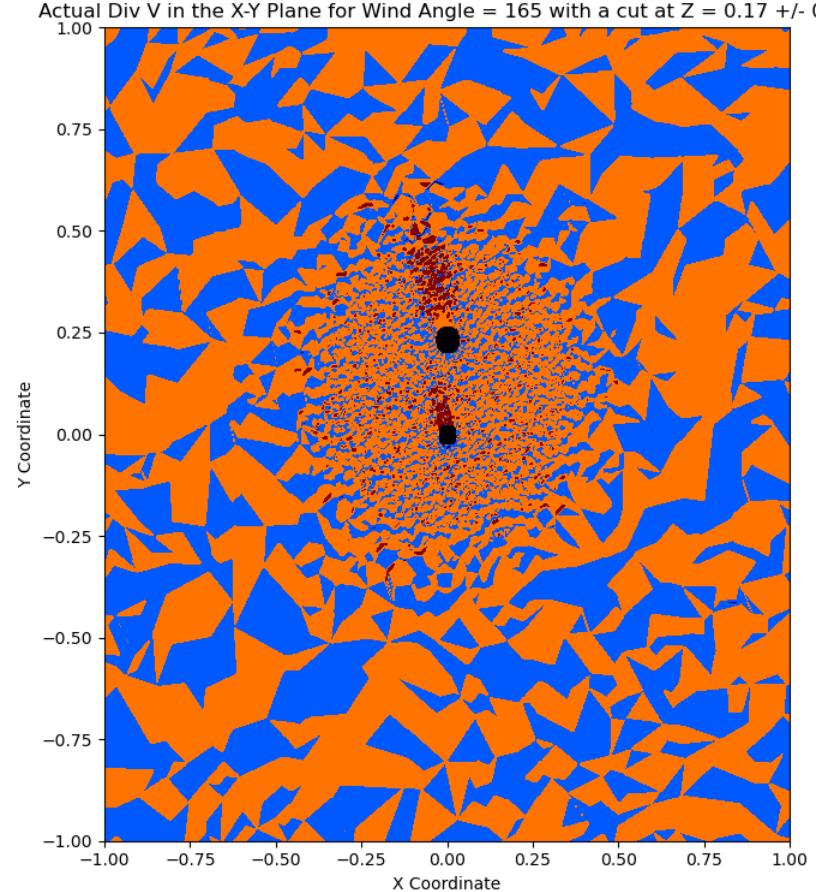
Comparison of Actual vs. Predicted values with Wind Angle = 150 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



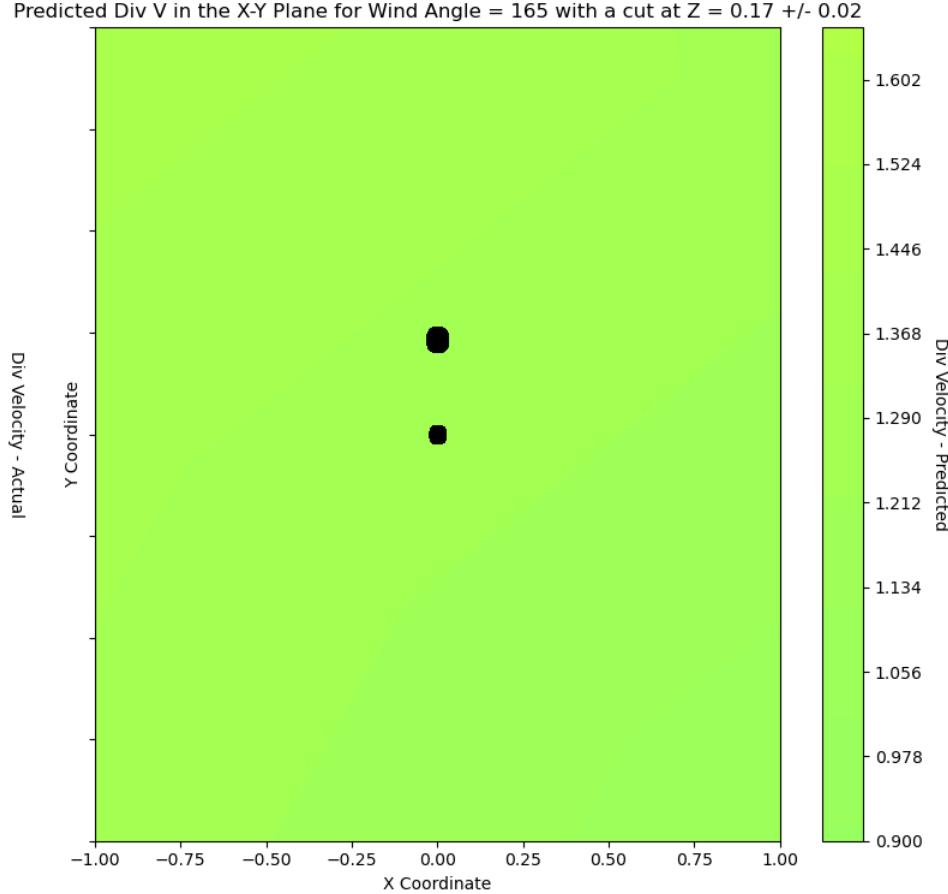
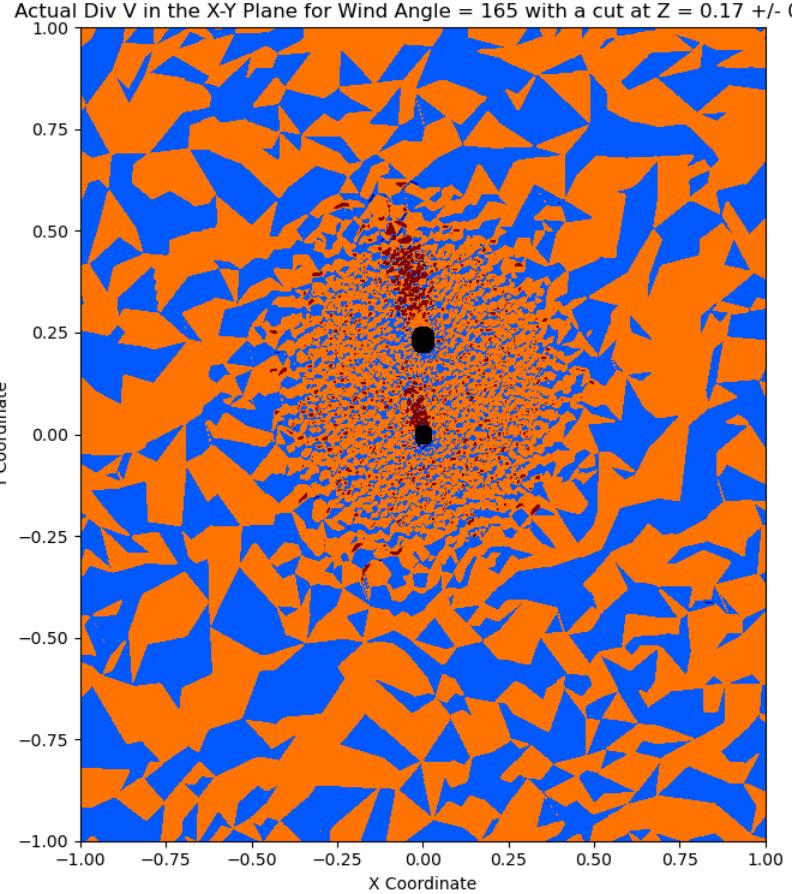
Comparison of Actual vs. Predicted values with Wind Angle = 150 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



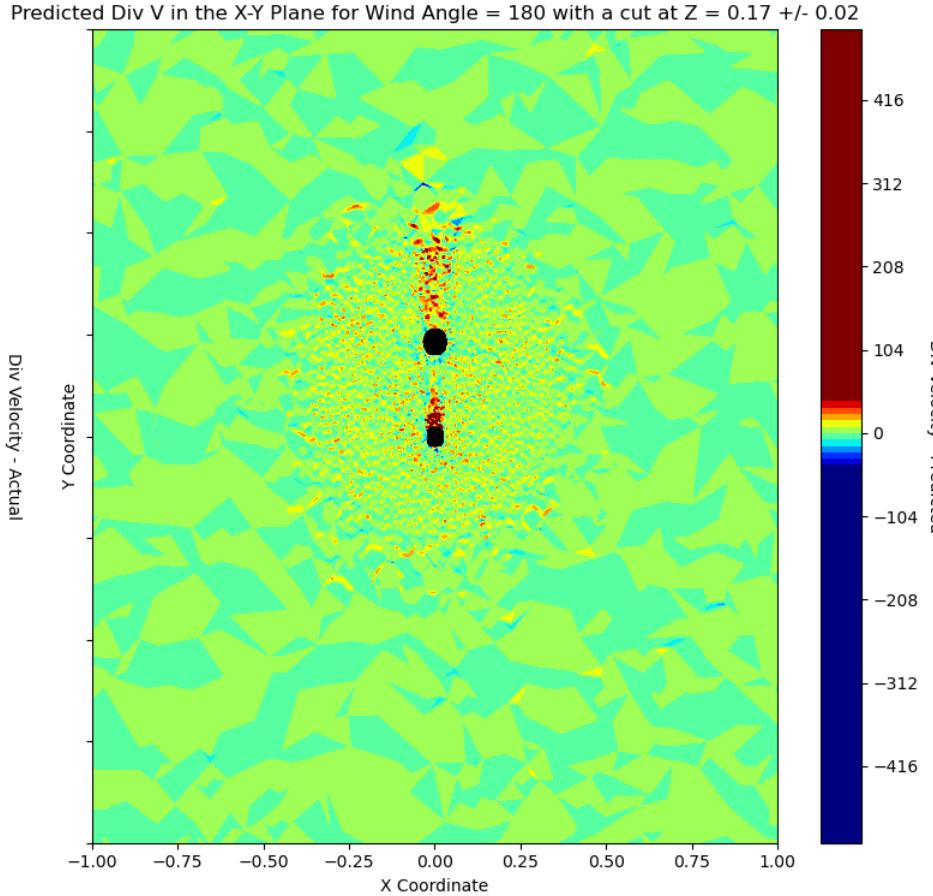
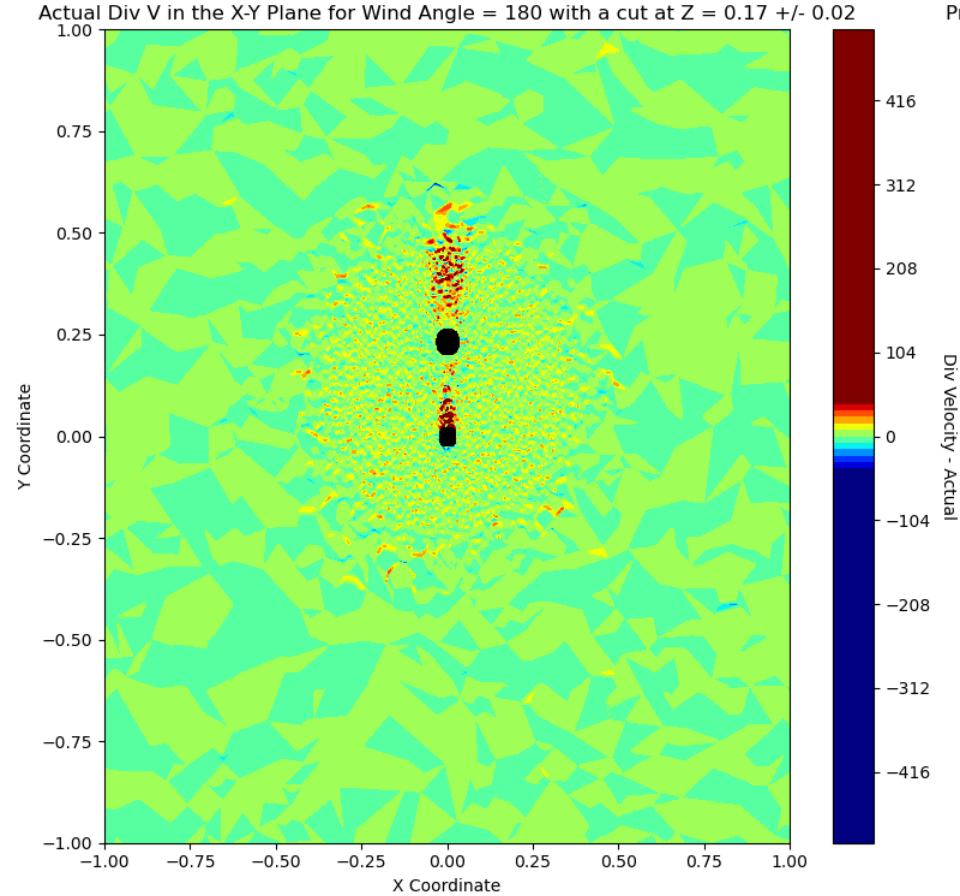
Comparison of Actual vs. Predicted values with Wind Angle = 165 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



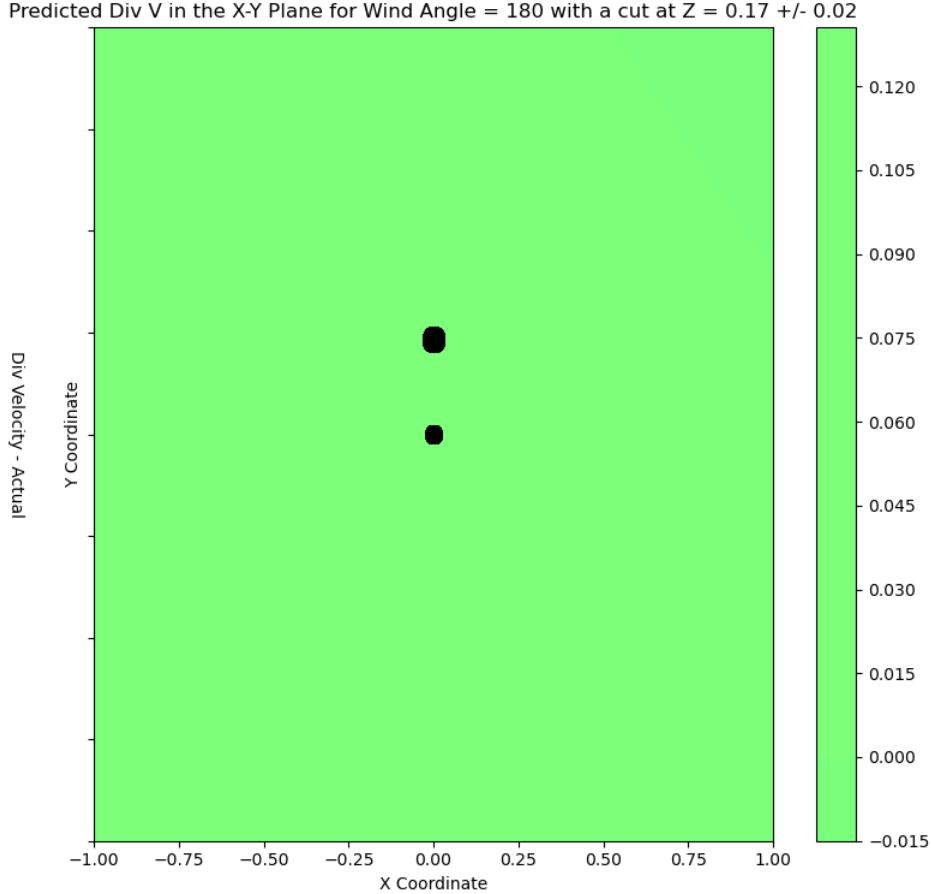
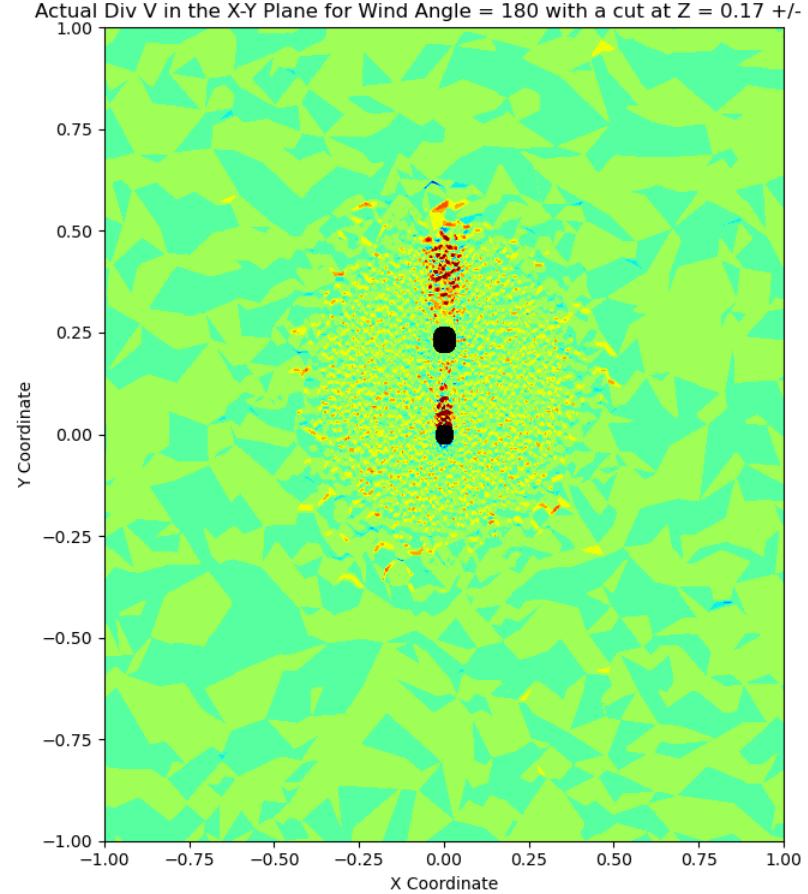
Comparison of Actual vs. Predicted values with Wind Angle = 165 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



Comparison of Actual vs. Predicted values with Wind Angle = 180 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



Comparison of Actual vs. Predicted values with Wind Angle = 180 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02

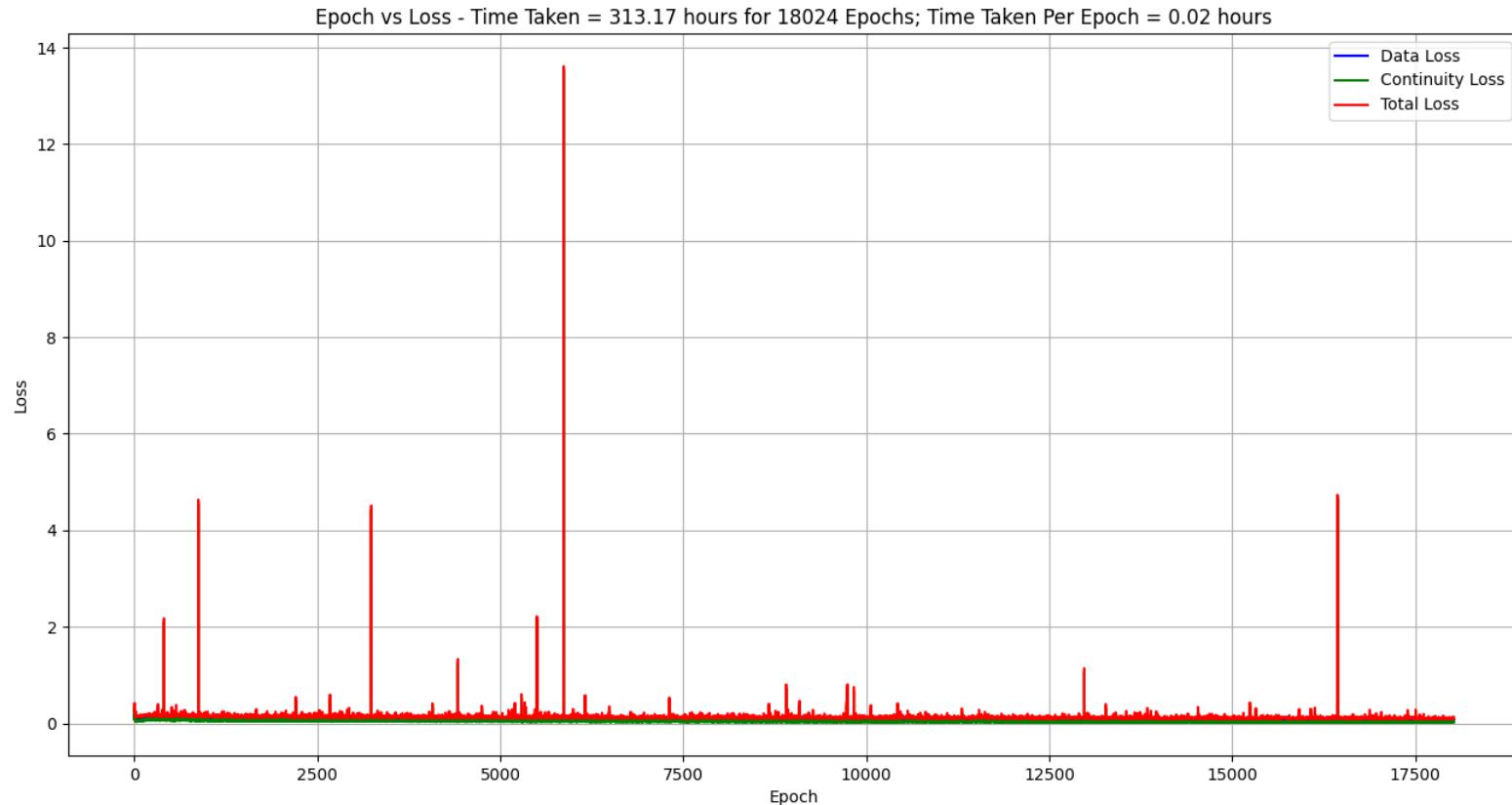


Progress so far - Data + Cont Loss  
Standard Normal Scalar, Adaptive Weighting  
(Adam Optimizer)

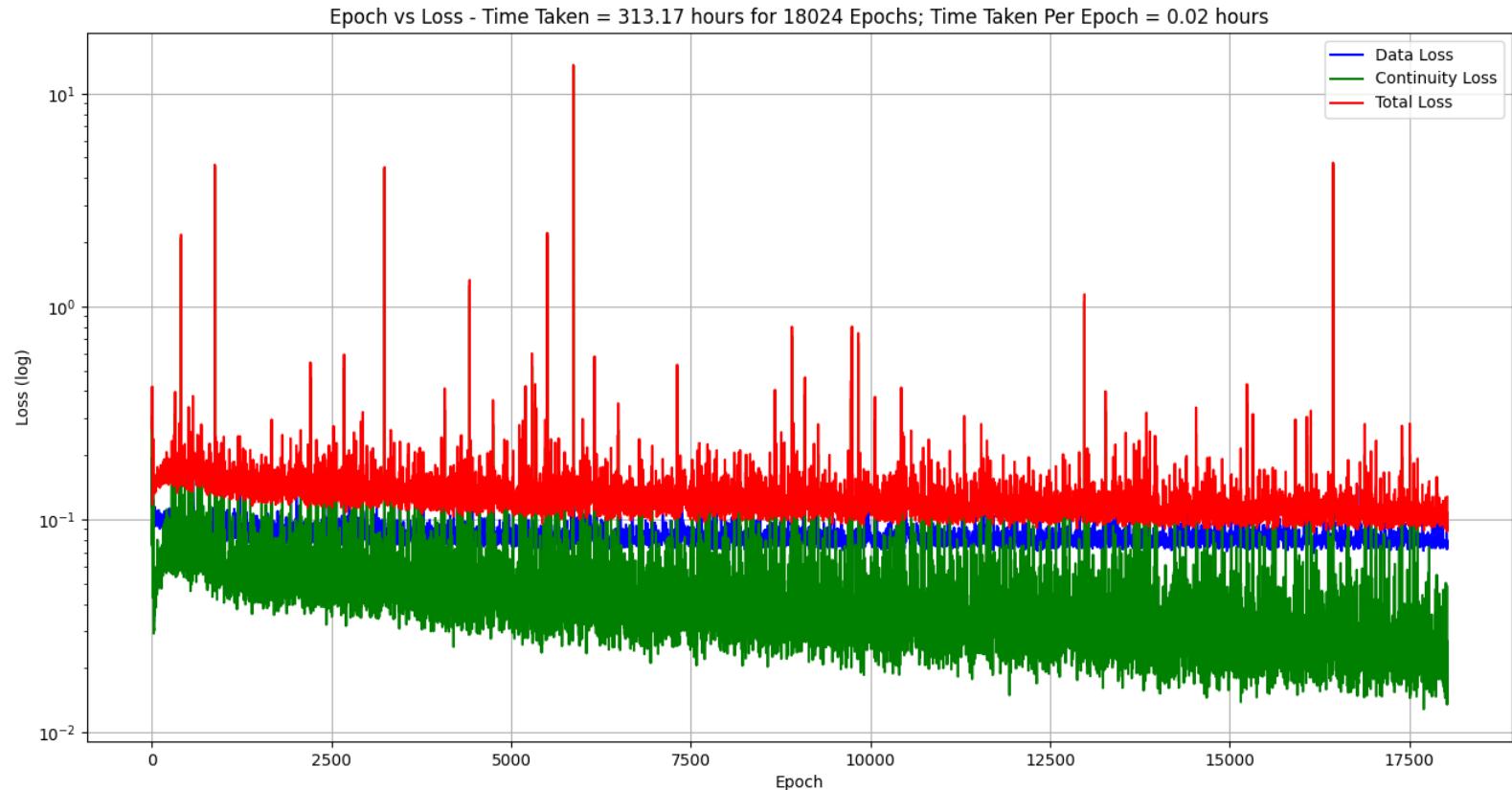
Threshold = 1E-5 (18012 Epochs, not completed), GPU Laptop

Scripts v4 – PREDICTING (135 DEG)

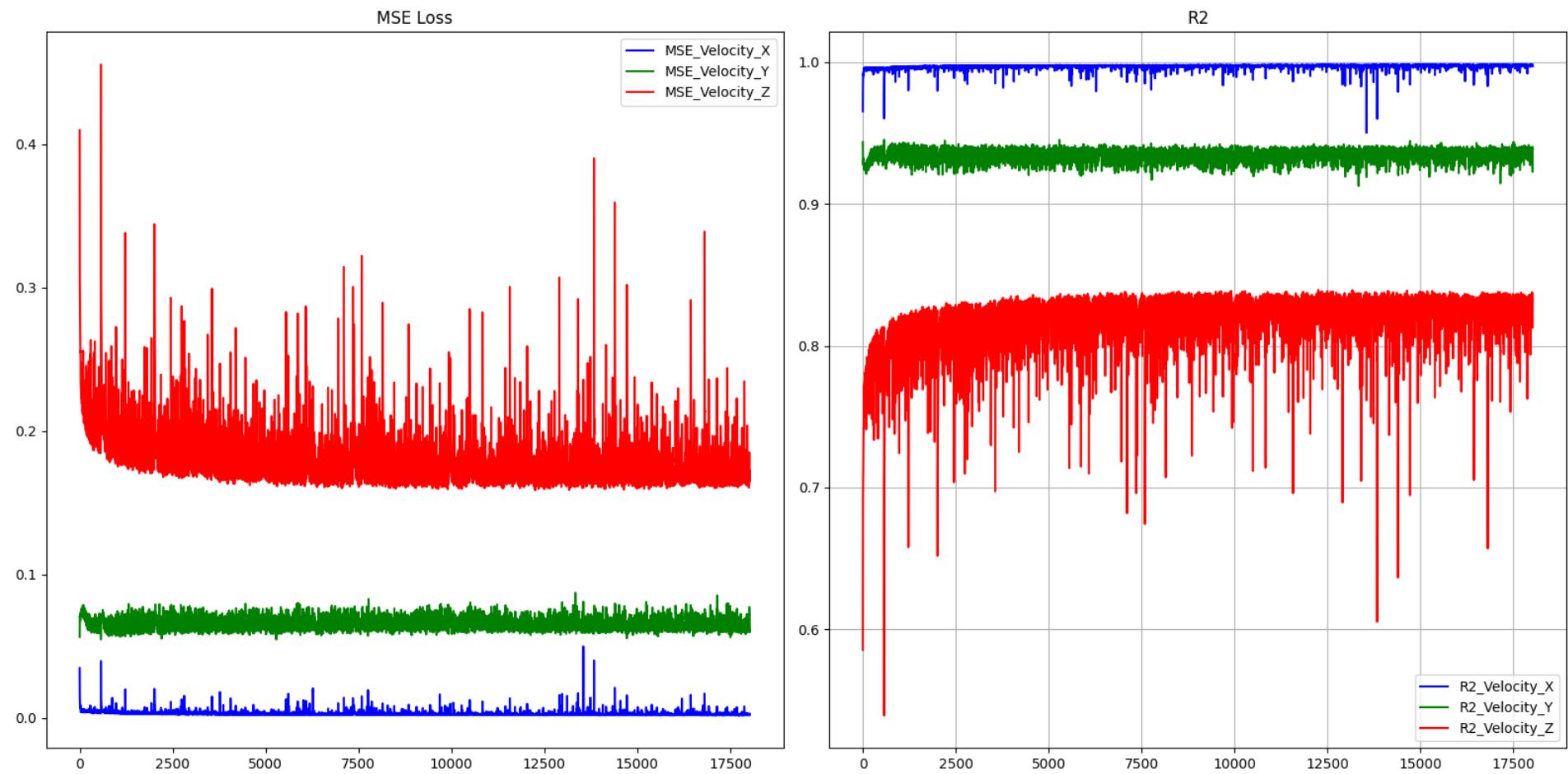
Progress so far - Data + Cont Loss (Adam Optimizer – Std Normal Scalar, Adaptive Weighting)  
Logging Plots (Training)



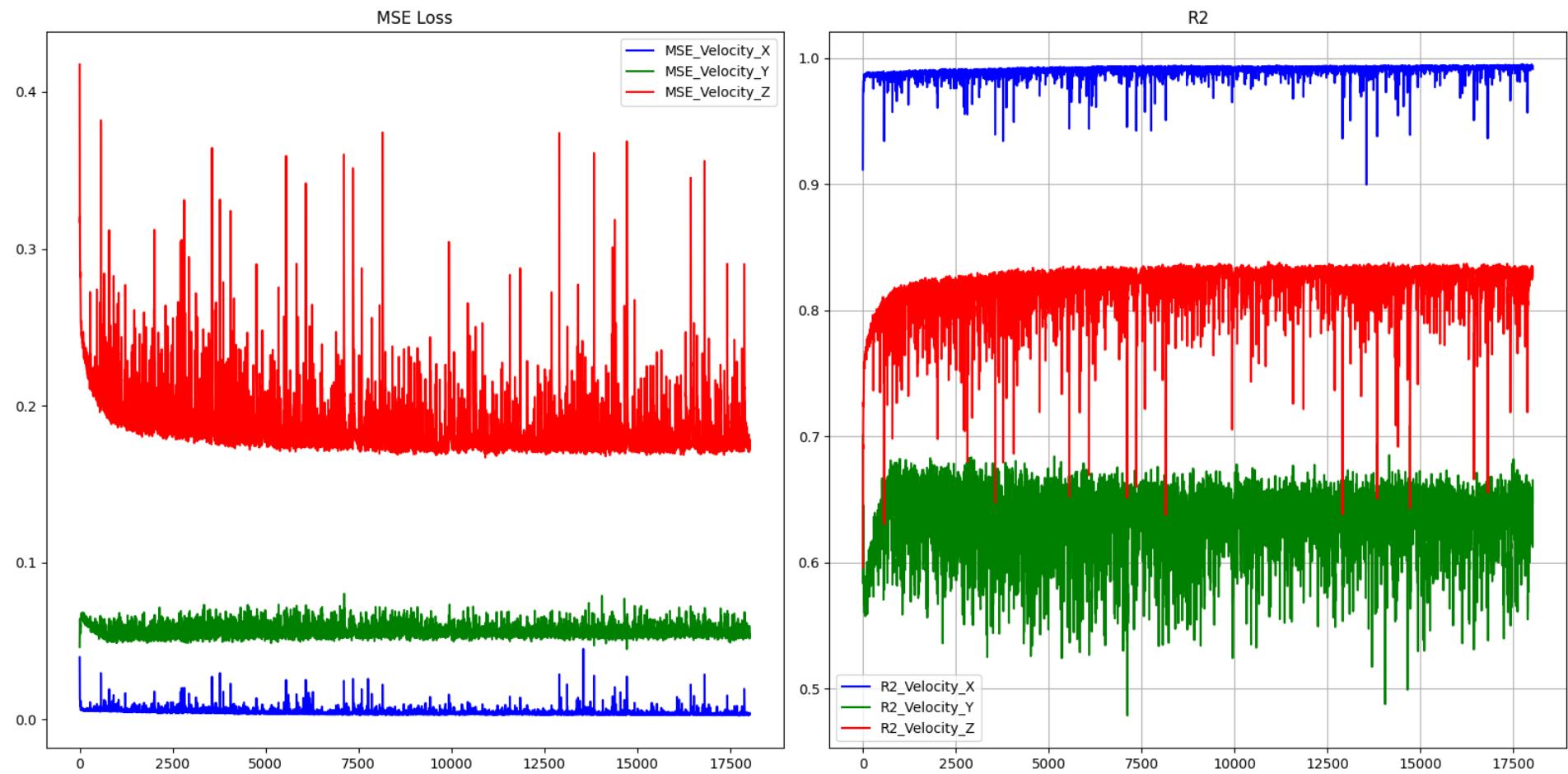
Progress so far - Data + Cont Loss (Adam Optimizer – Std Normal Scalar, Adaptive Weighting)  
Logging Plots (Training)



Progress so far - Data + Cont Loss (Adam Optimizer – Std Normal Scalar, Adaptive Weighting)  
Logging Plots (Testing)



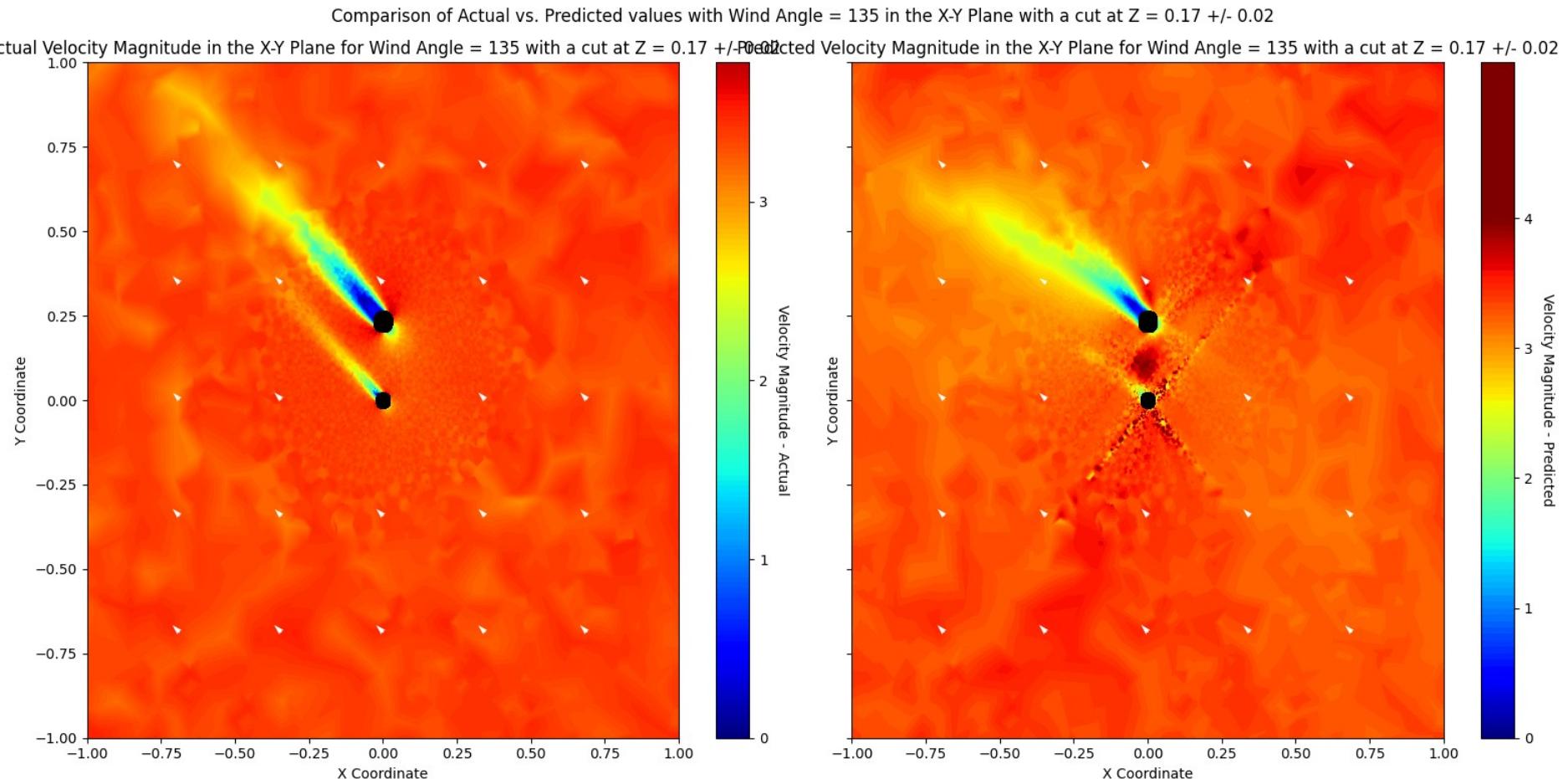
Progress so far - Data + Cont Loss (Adam Optimizer – Std Normal Scalar, Adaptive Weighting)  
Logging Plots (Predicting 135)



Progress so far - Data + Cont Loss - Adaptive Weighting  
Threshold = SMA1E-5 (18012 Epochs, not completed)  
Predicting Results – Metrics (Angle = 135)

Variable	MSE	RMSE	MAE	R2
Velocity:0	0.0067679894550453	0.0822677911156326	0.0556955966133766	0.993359685332148
Velocity:1	0.351886210856887	0.593199975435676	0.285545116212183	0.658043452264219
Velocity:2	0.00555580049751874	0.0745372423525229	0.0328389109818245	0.830170865507425

Progress so far - Data + Cont Loss - Adaptive Weighting  
Threshold = SMA1E-5 (18012 Epochs, not completed)

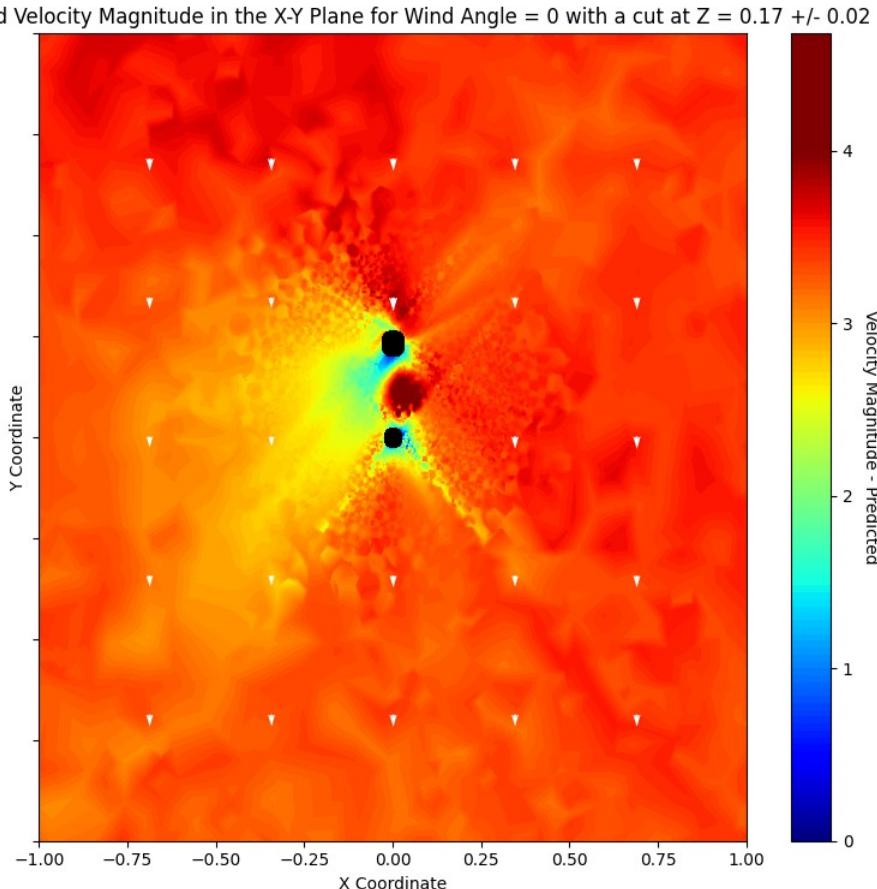
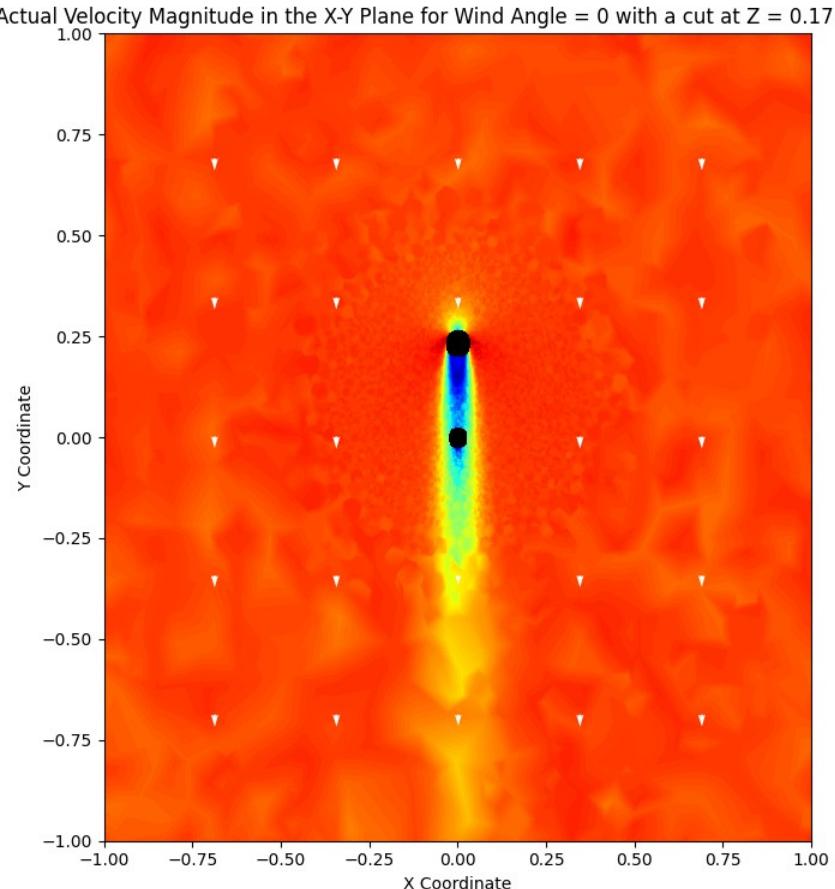


Progress so far - Data + Cont Loss  
Standard Normal Scalar, Adaptive Weighting  
(Adam Optimizer)

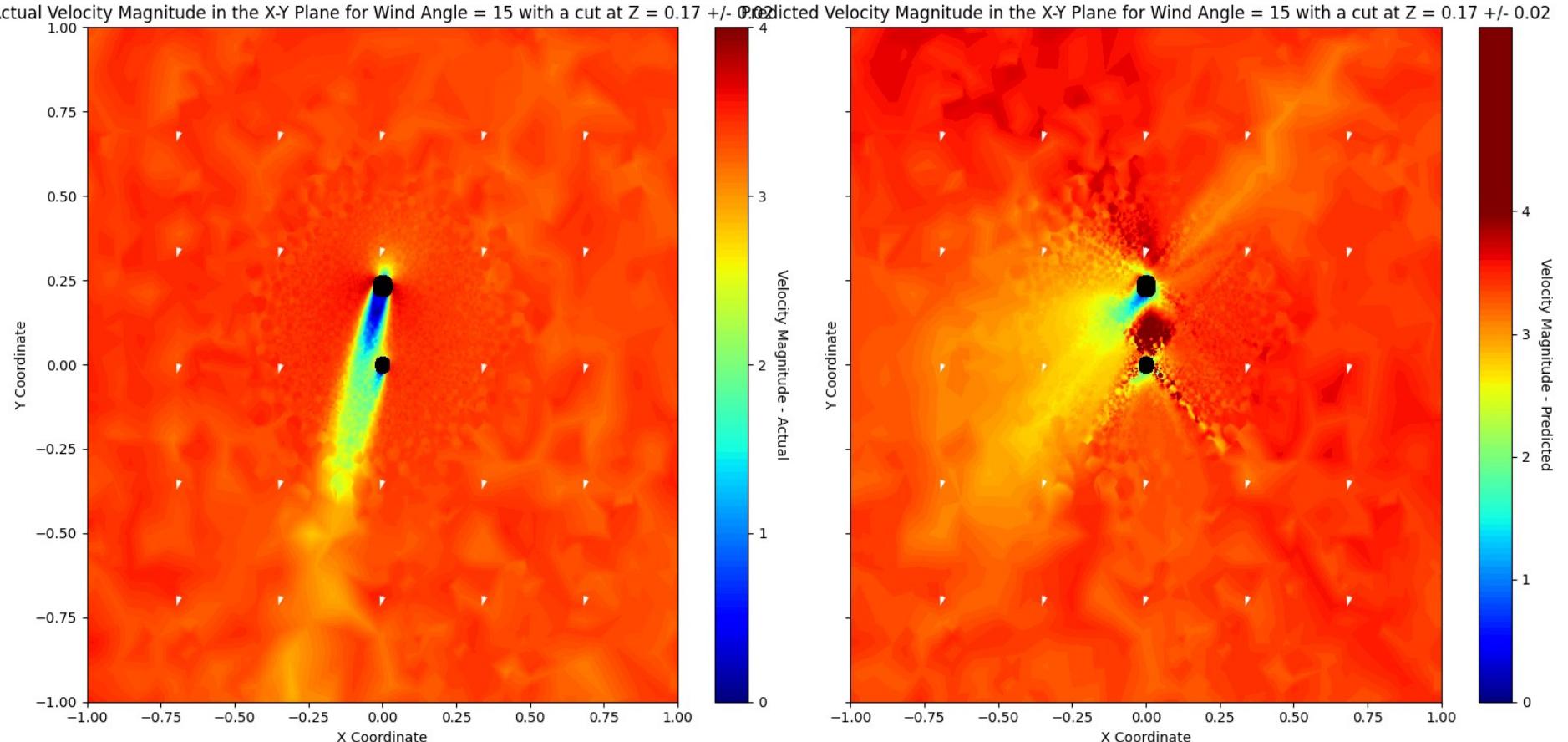
Threshold = SMA1E-5 (18012 Epochs, not completed), GPU Laptop

Scripts v4 – TESTING

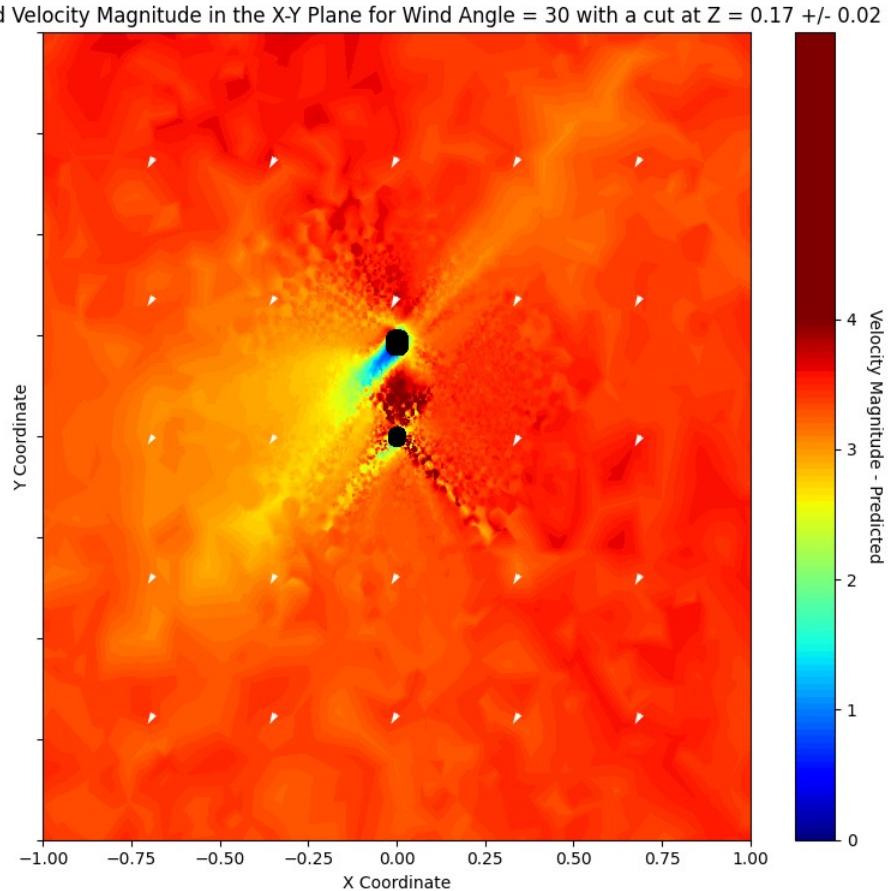
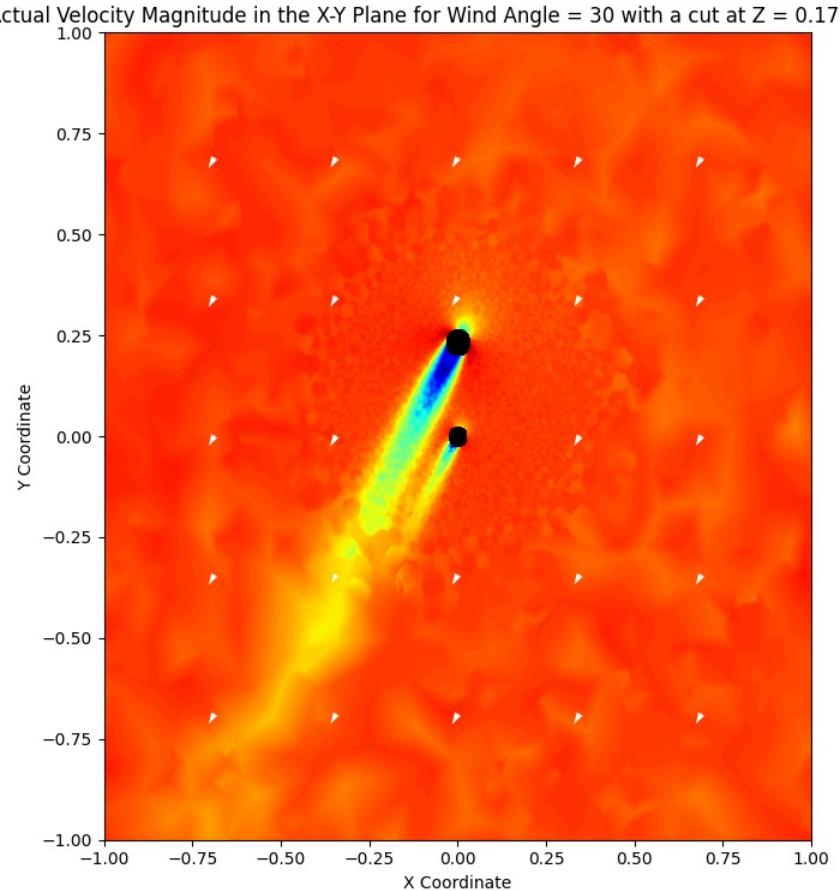
Comparison of Actual vs. Predicted values with Wind Angle = 0 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



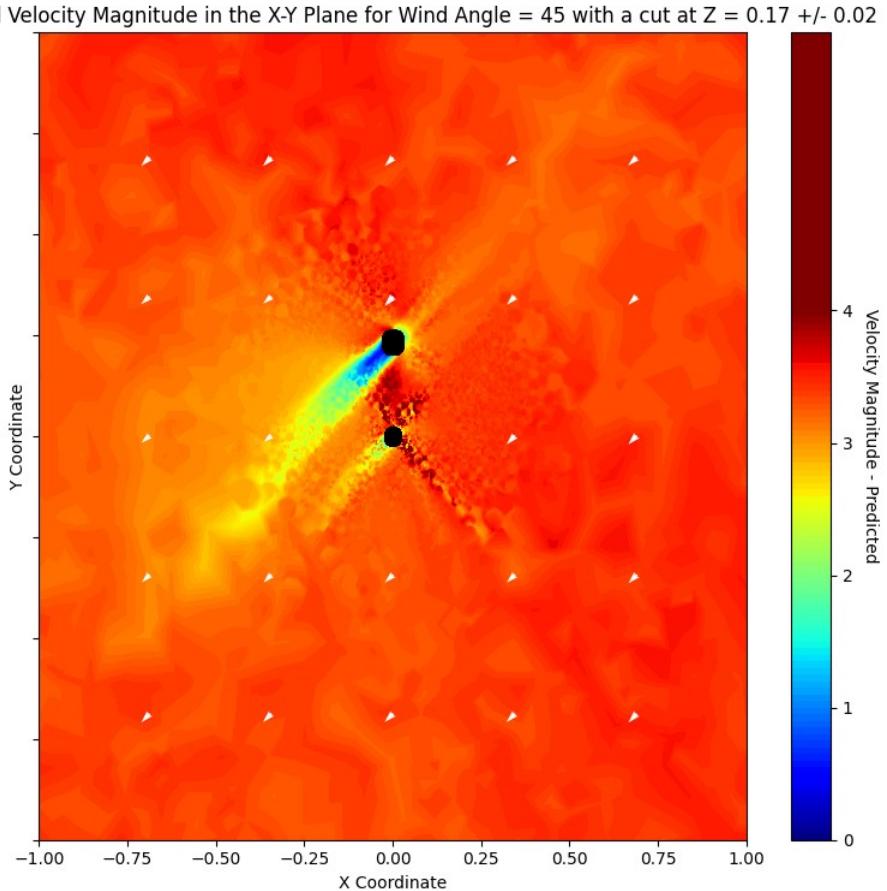
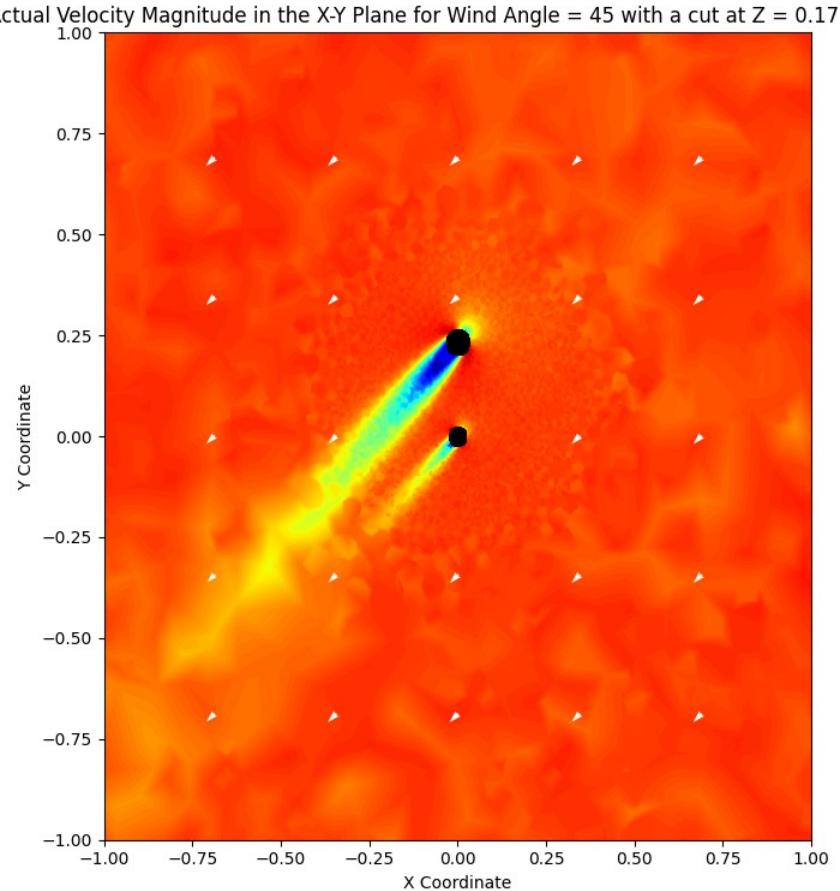
Comparison of Actual vs. Predicted values with Wind Angle = 15 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



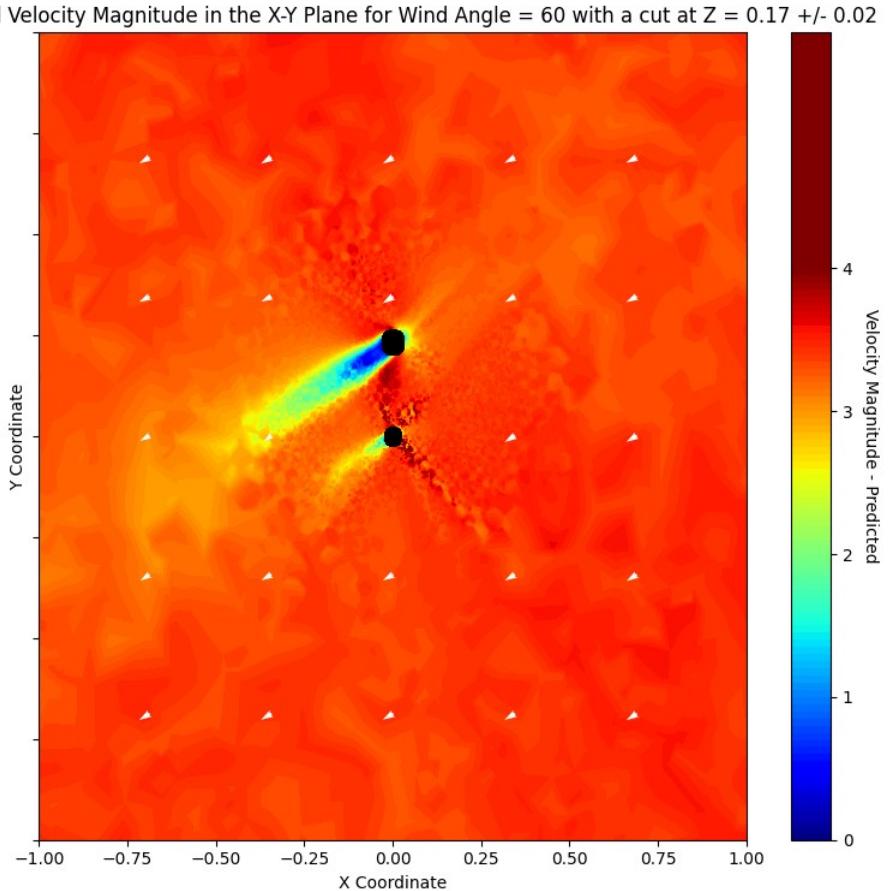
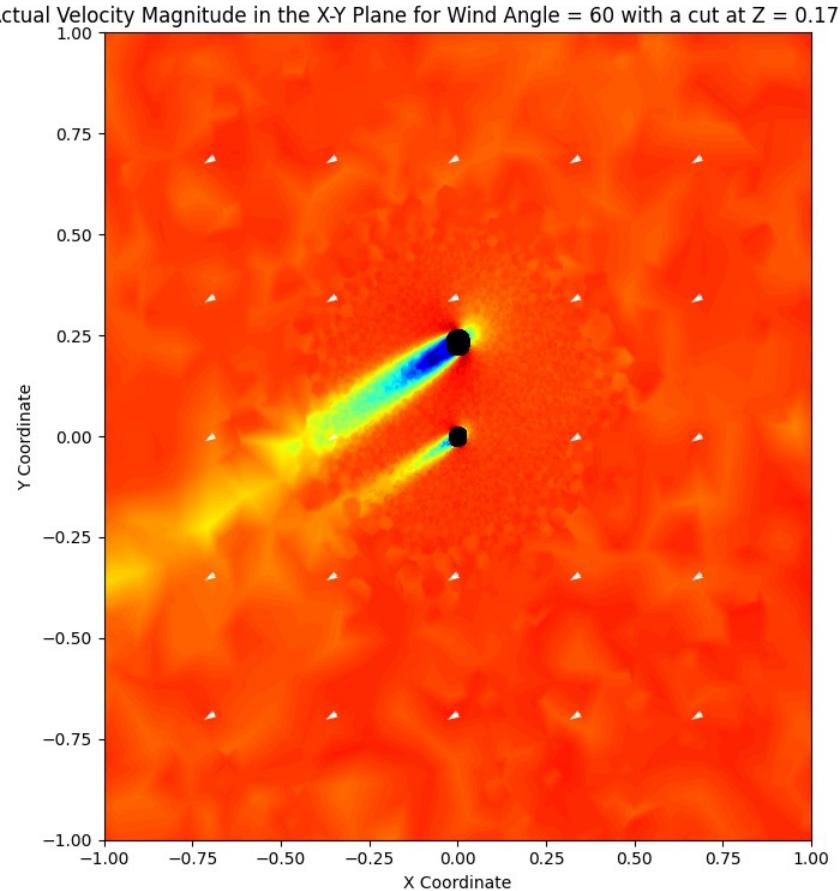
Comparison of Actual vs. Predicted values with Wind Angle = 30 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



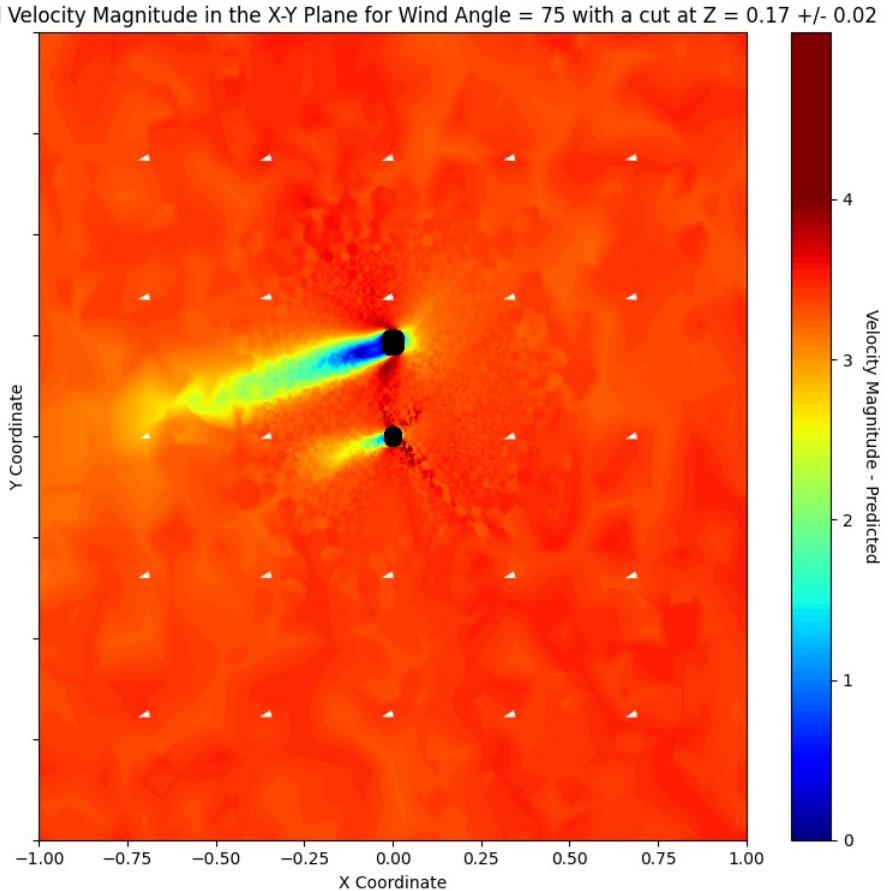
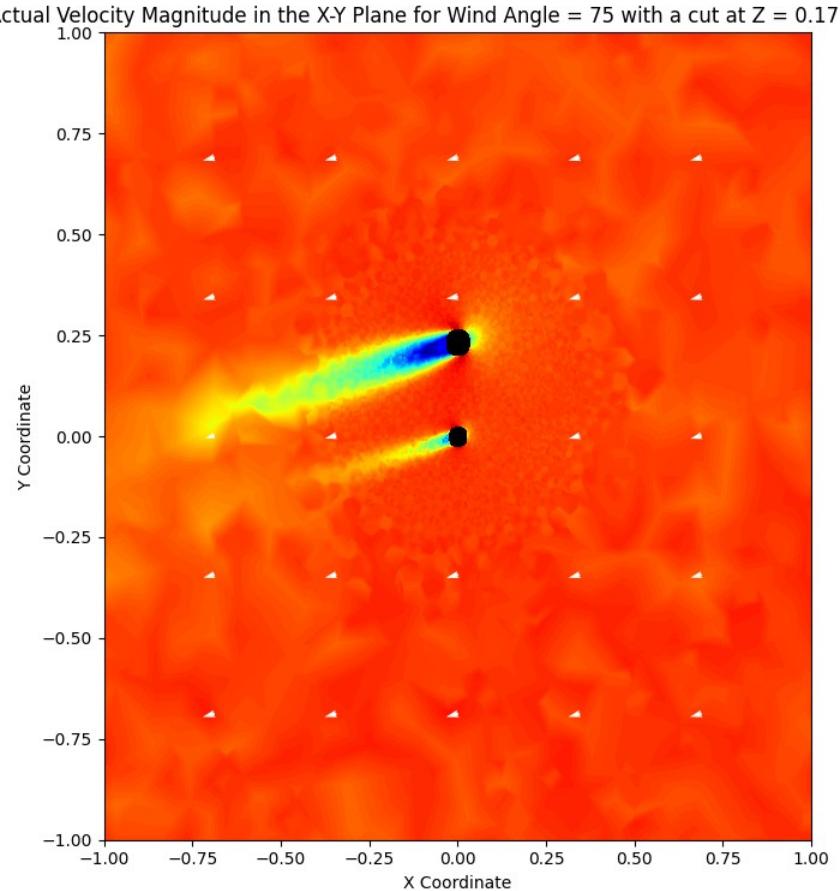
Comparison of Actual vs. Predicted values with Wind Angle = 45 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



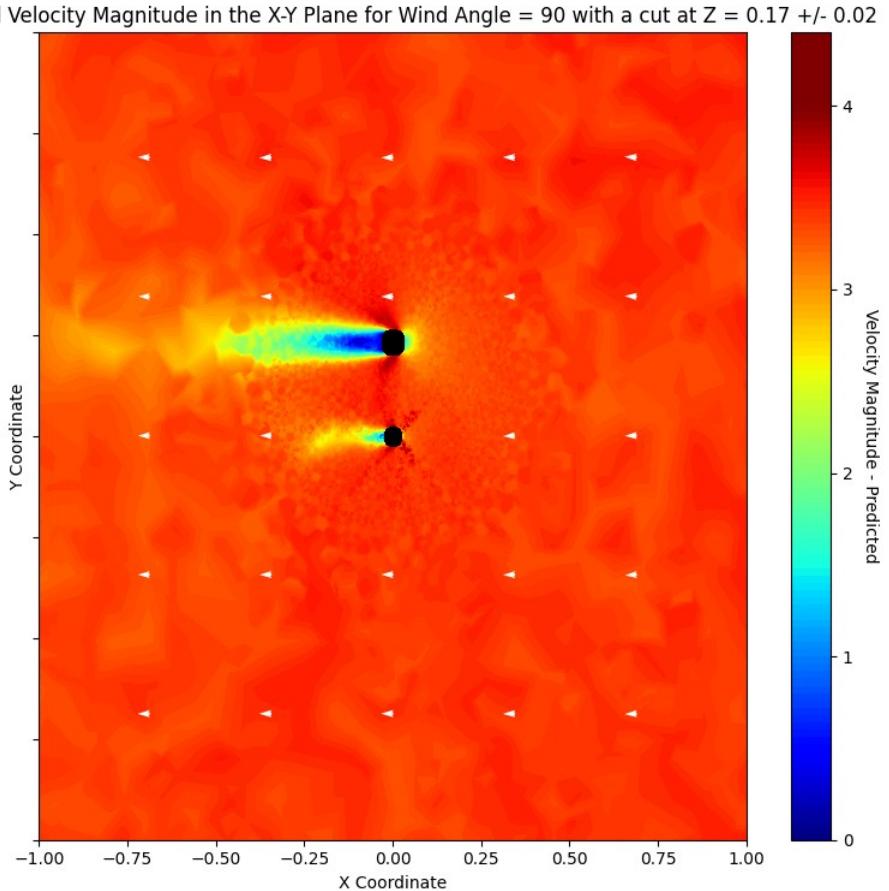
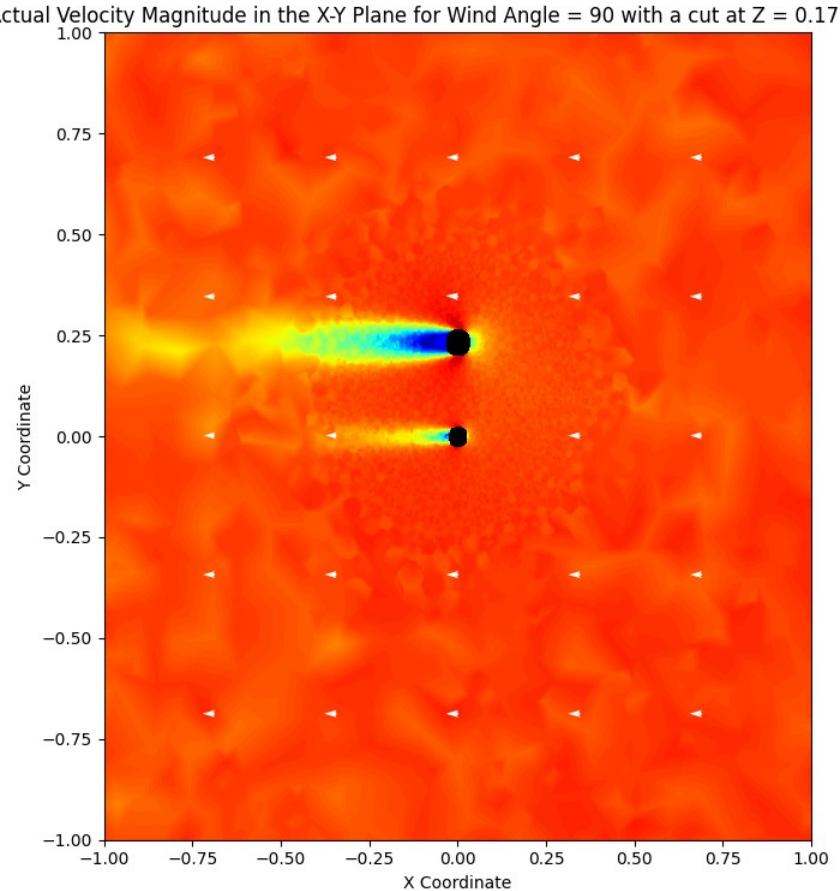
Comparison of Actual vs. Predicted values with Wind Angle = 60 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



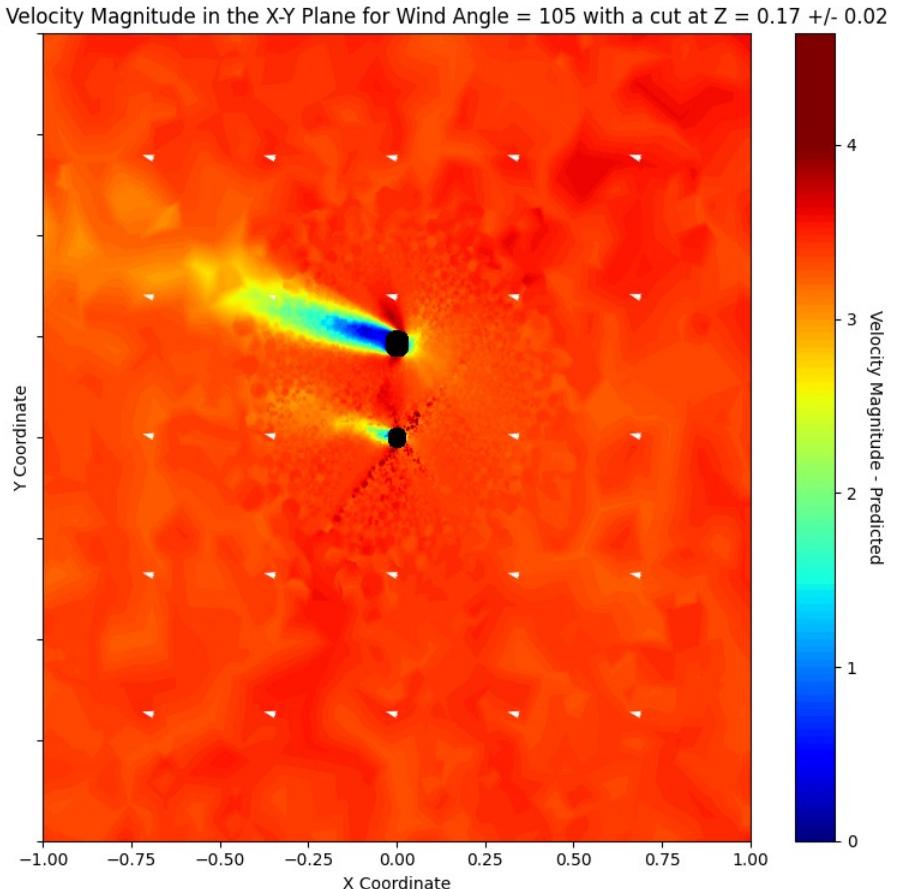
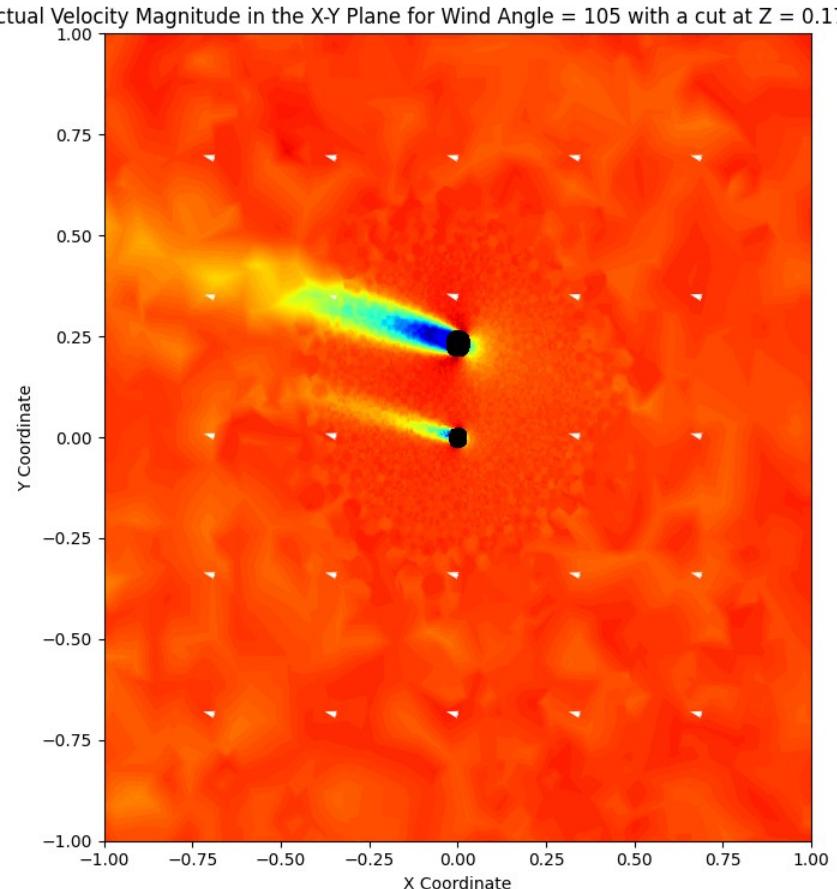
Comparison of Actual vs. Predicted values with Wind Angle = 75 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



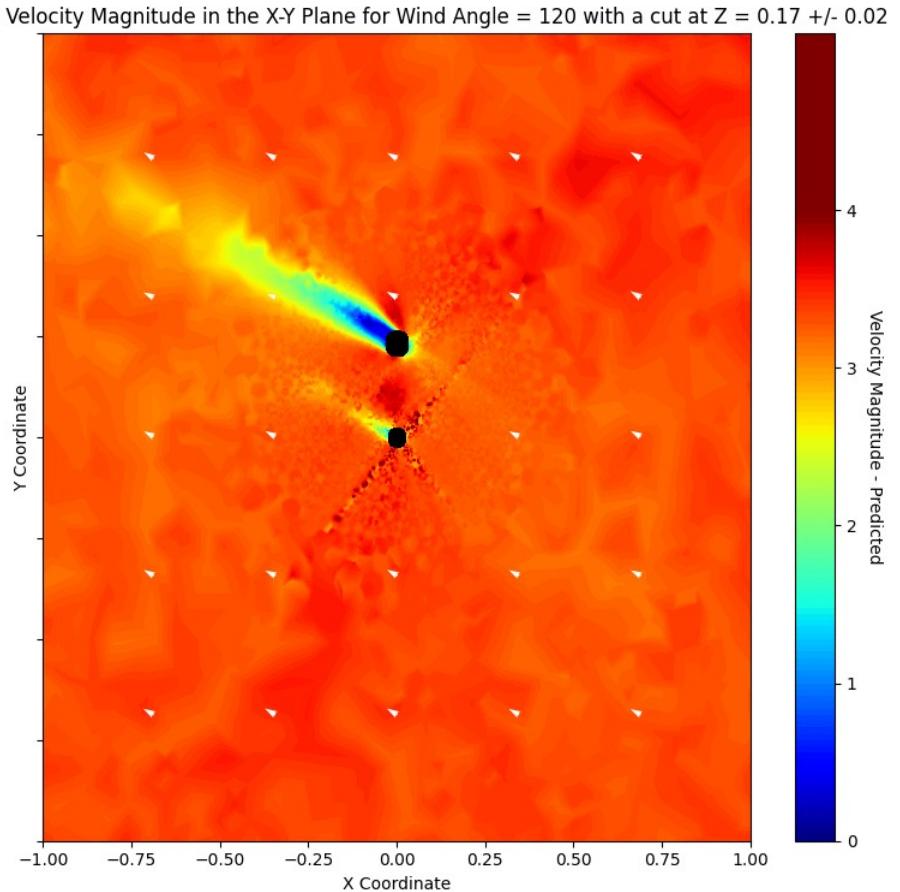
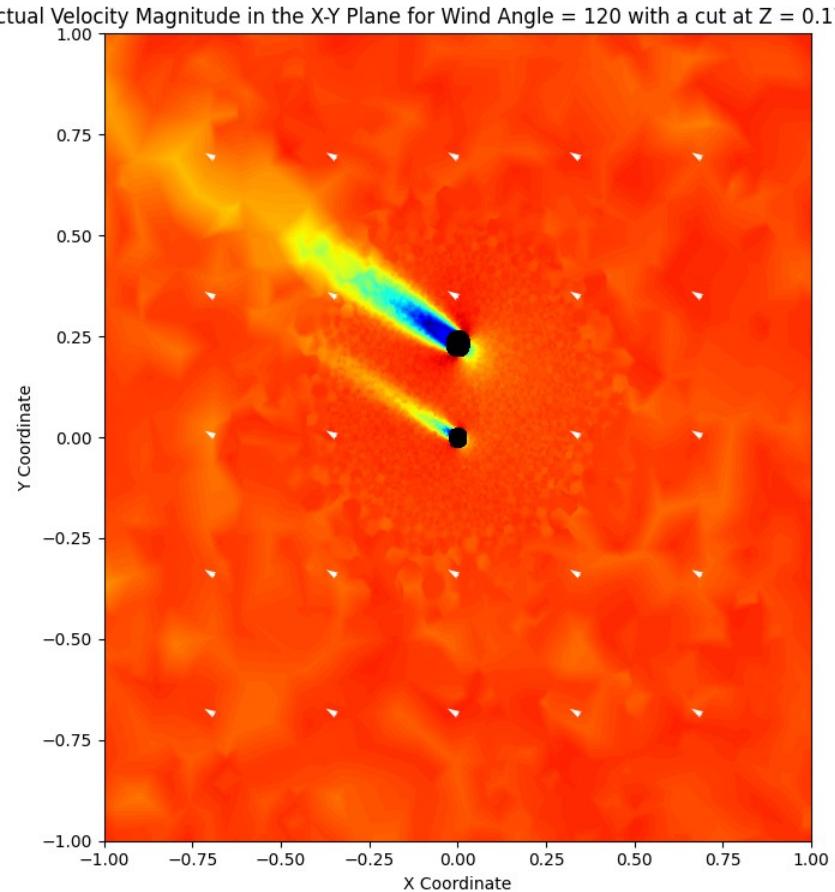
Comparison of Actual vs. Predicted values with Wind Angle = 90 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



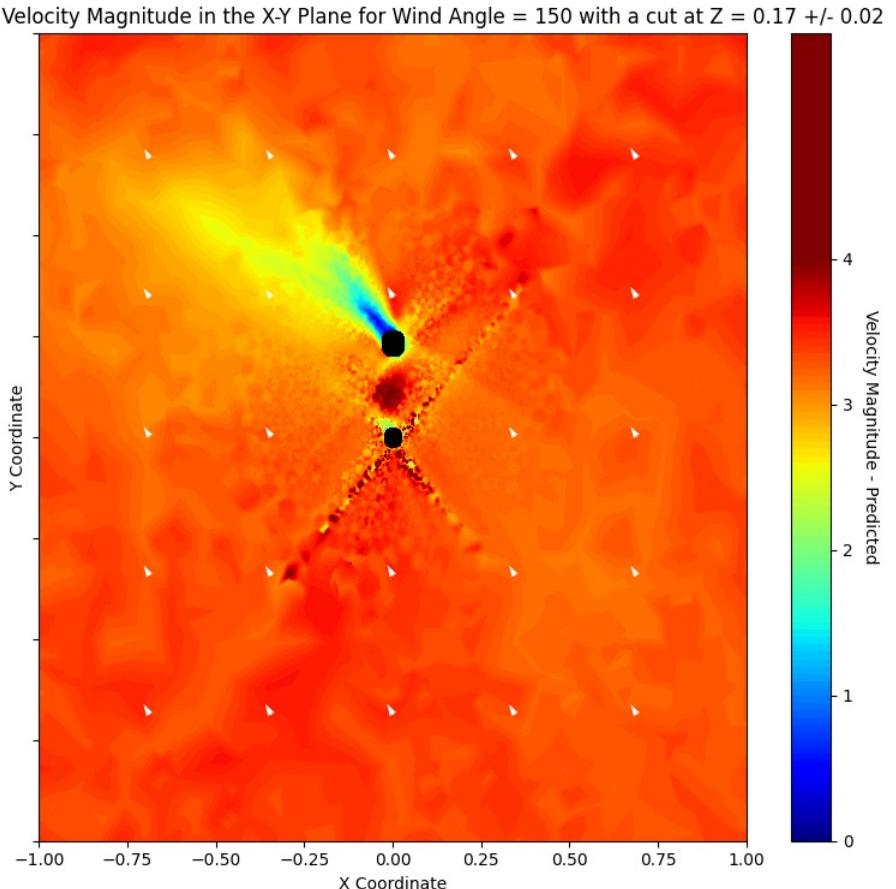
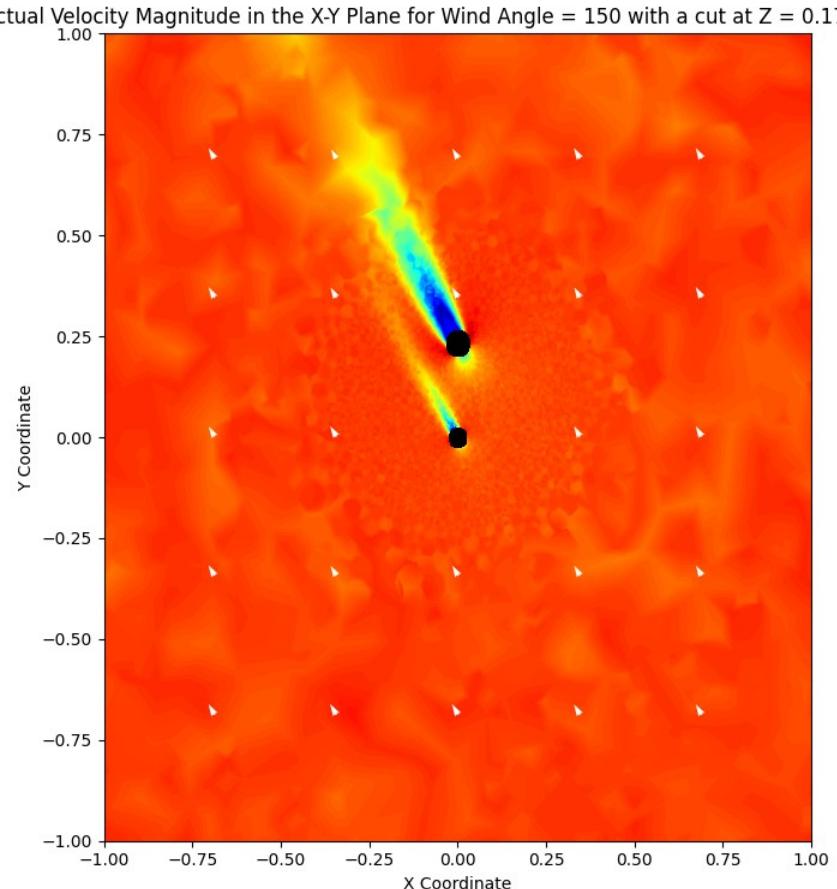
Comparison of Actual vs. Predicted values with Wind Angle = 105 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



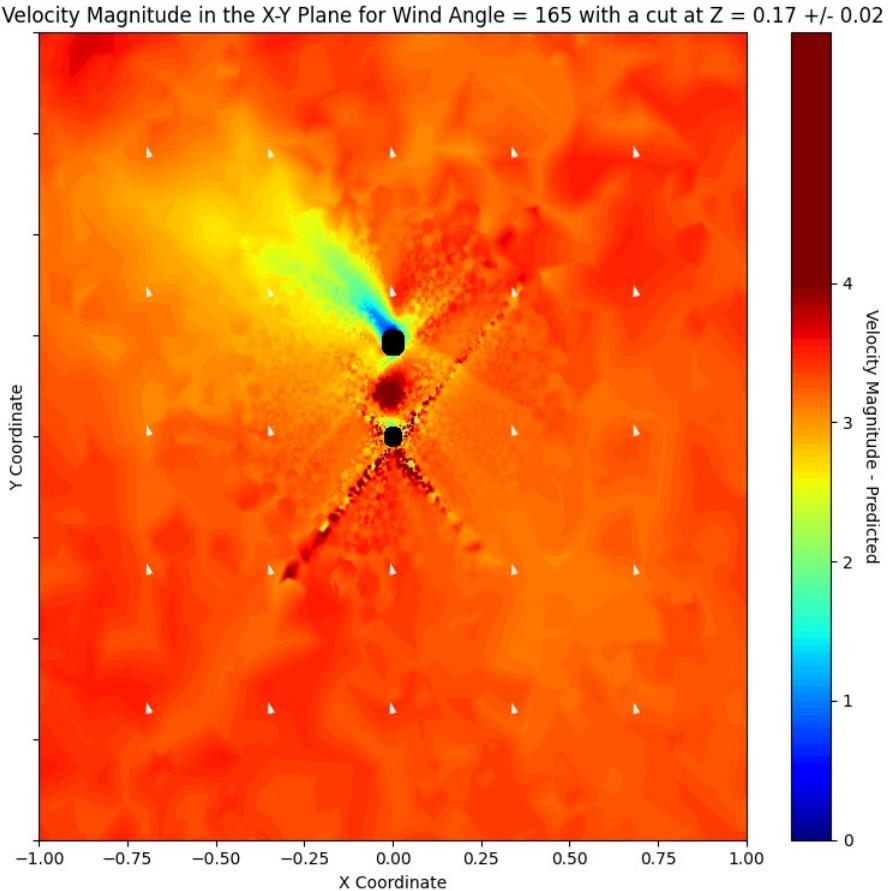
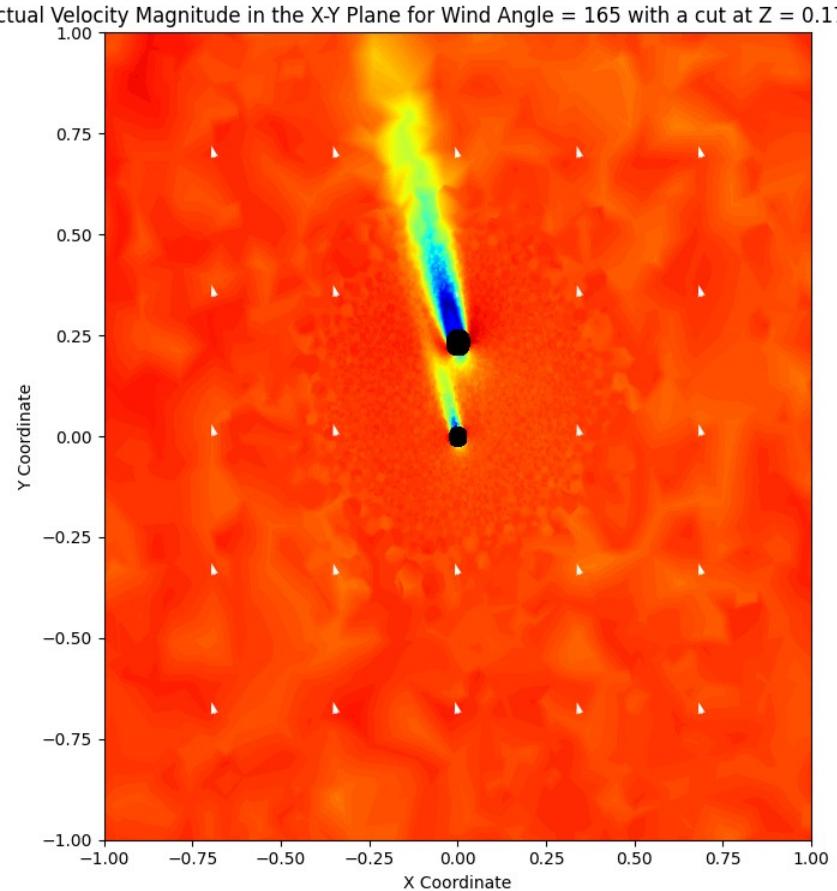
Comparison of Actual vs. Predicted values with Wind Angle = 120 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



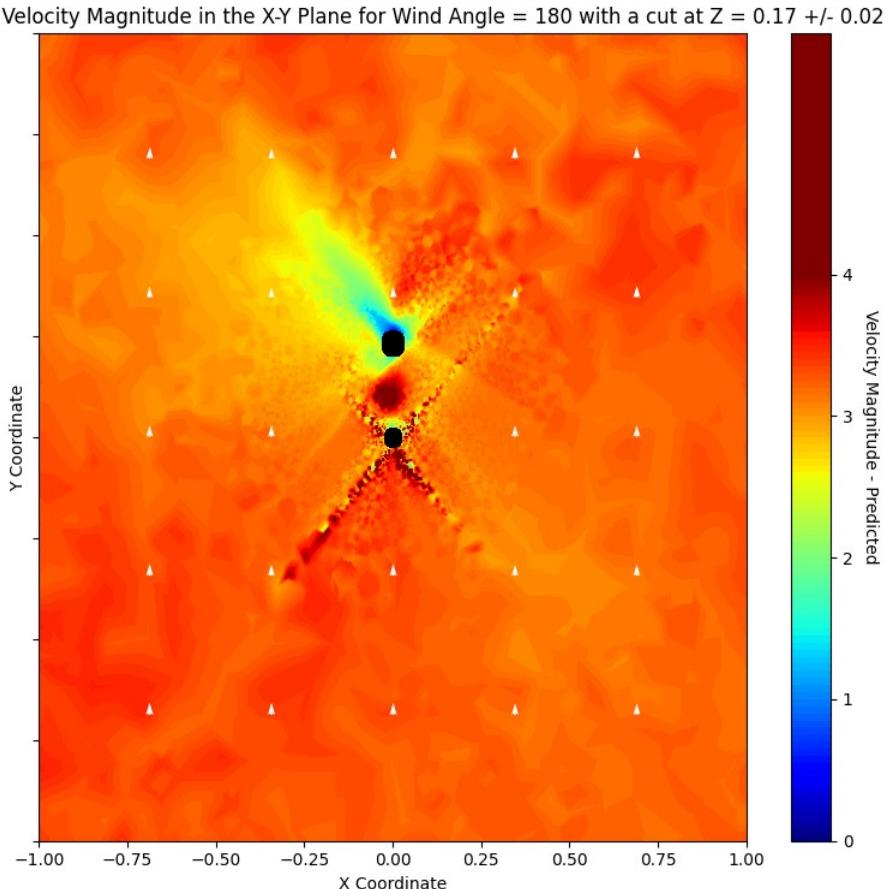
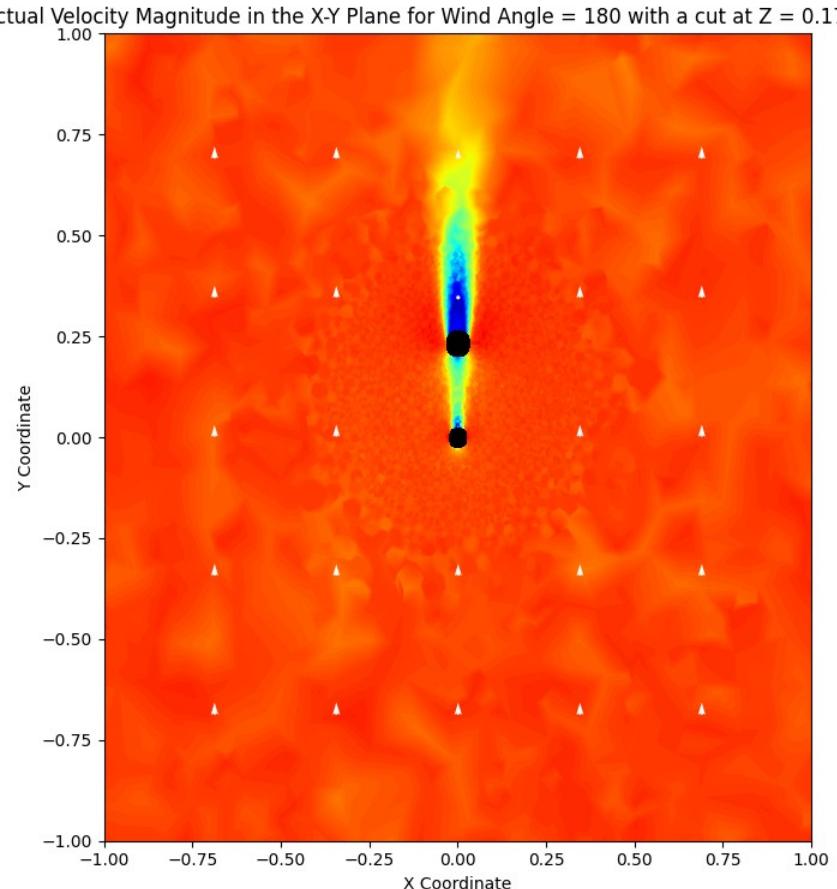
Comparison of Actual vs. Predicted values with Wind Angle = 150 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



Comparison of Actual vs. Predicted values with Wind Angle = 165 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



Comparison of Actual vs. Predicted values with Wind Angle = 180 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02

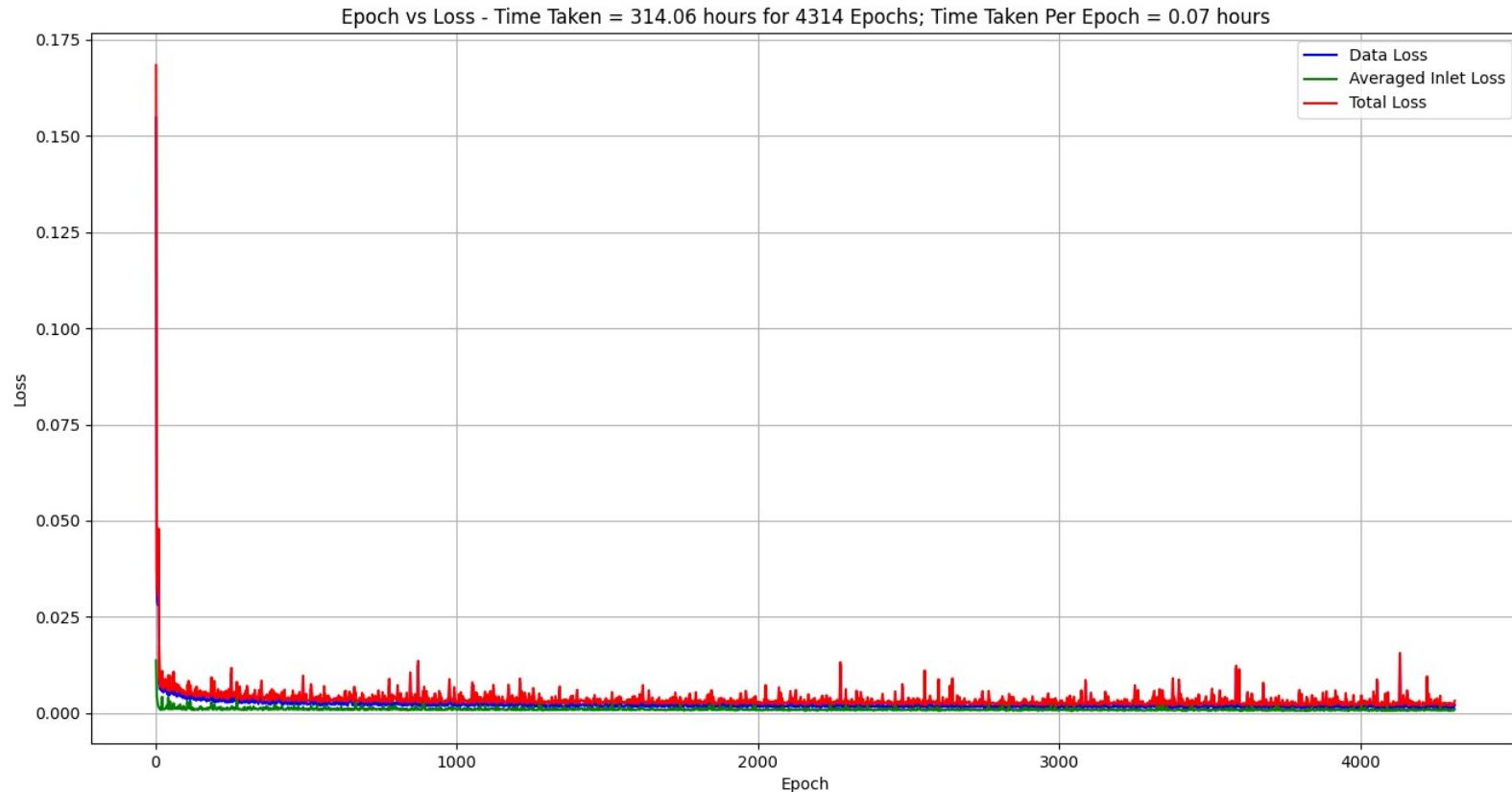


Progress so far - Data + Inlet Loss  
Standard Normal Scalar, Adaptive Weighting  
(Adam Optimizer)

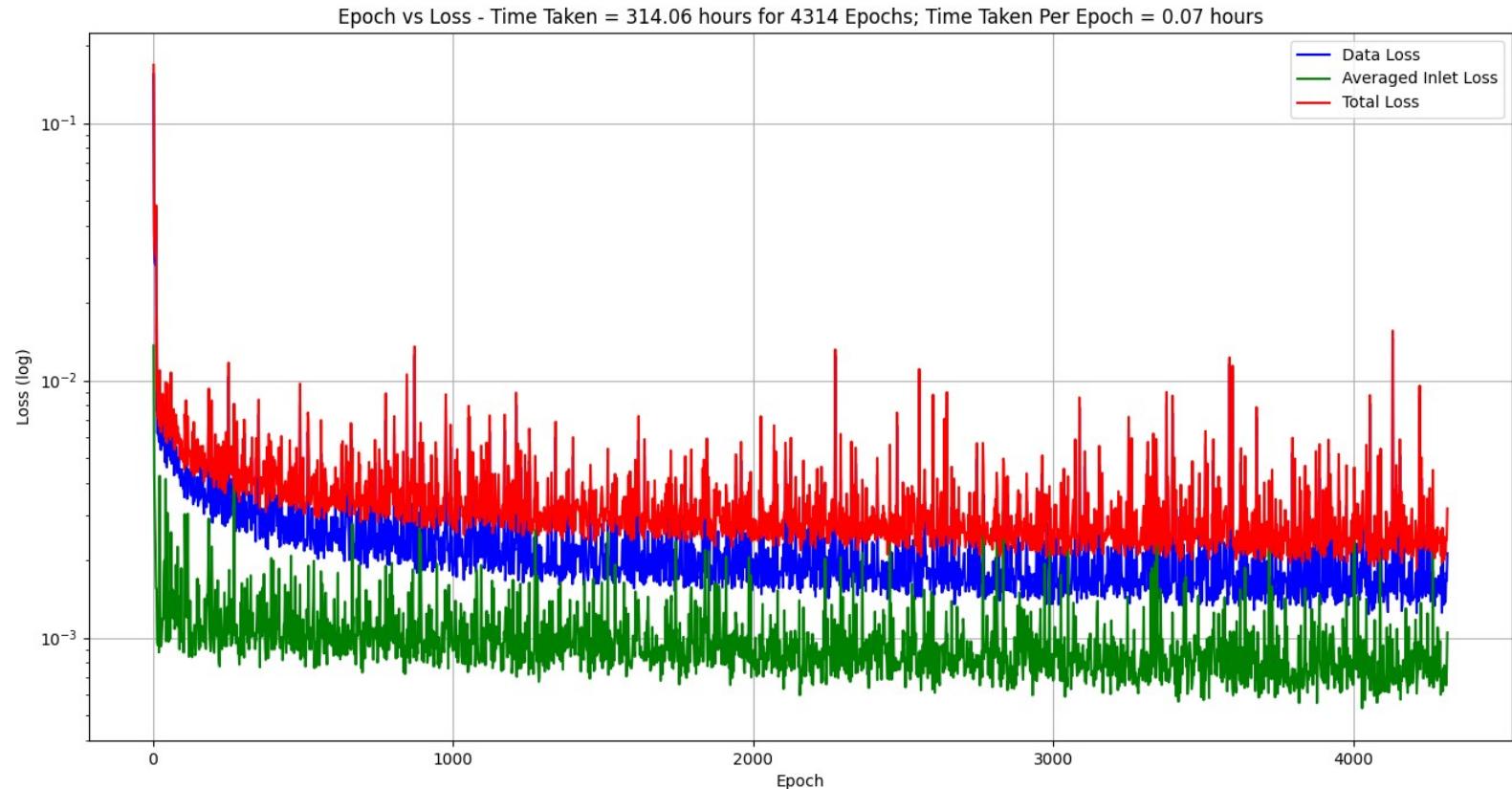
Threshold = 1E-5 (4314 Epochs, not completed), GPU Laptop

Scripts v4 – PREDICTING (135 DEG)

Progress so far - Data + Cont Loss (Adam Optimizer – Std Normal Scalar, Adaptive Weighting)  
Logging Plots (Training)

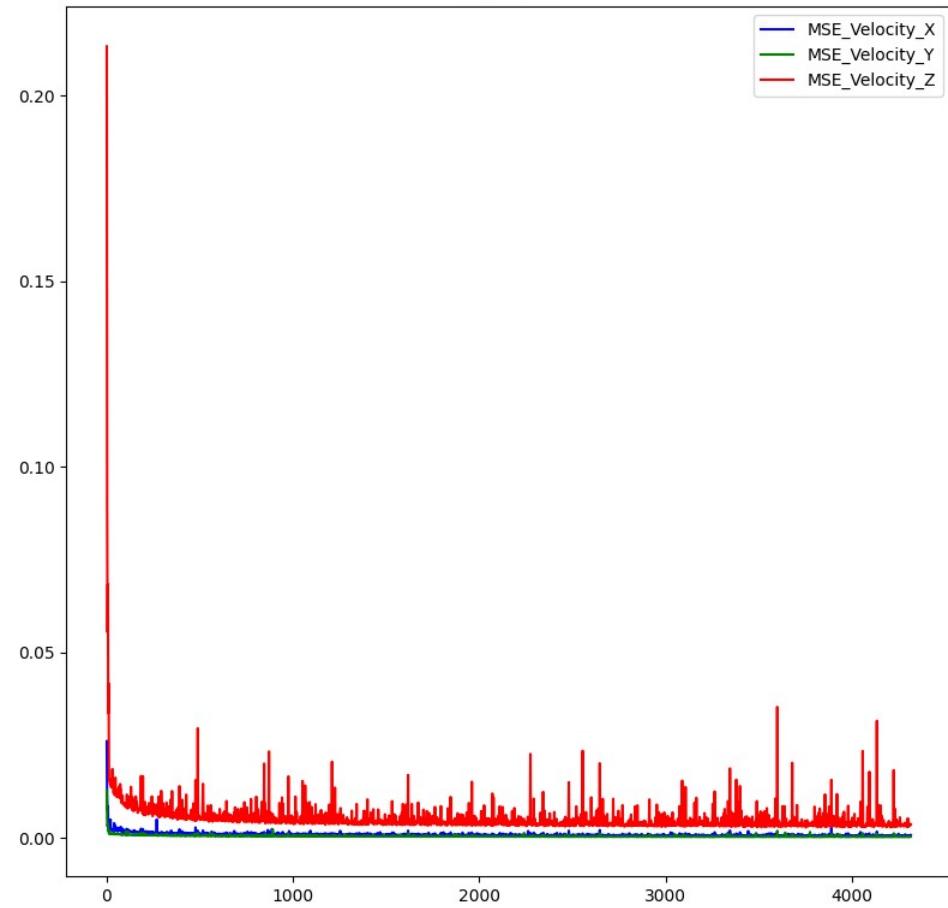


Progress so far - Data + Cont Loss (Adam Optimizer – Std Normal Scalar, Adaptive Weighting)  
Logging Plots (Training)

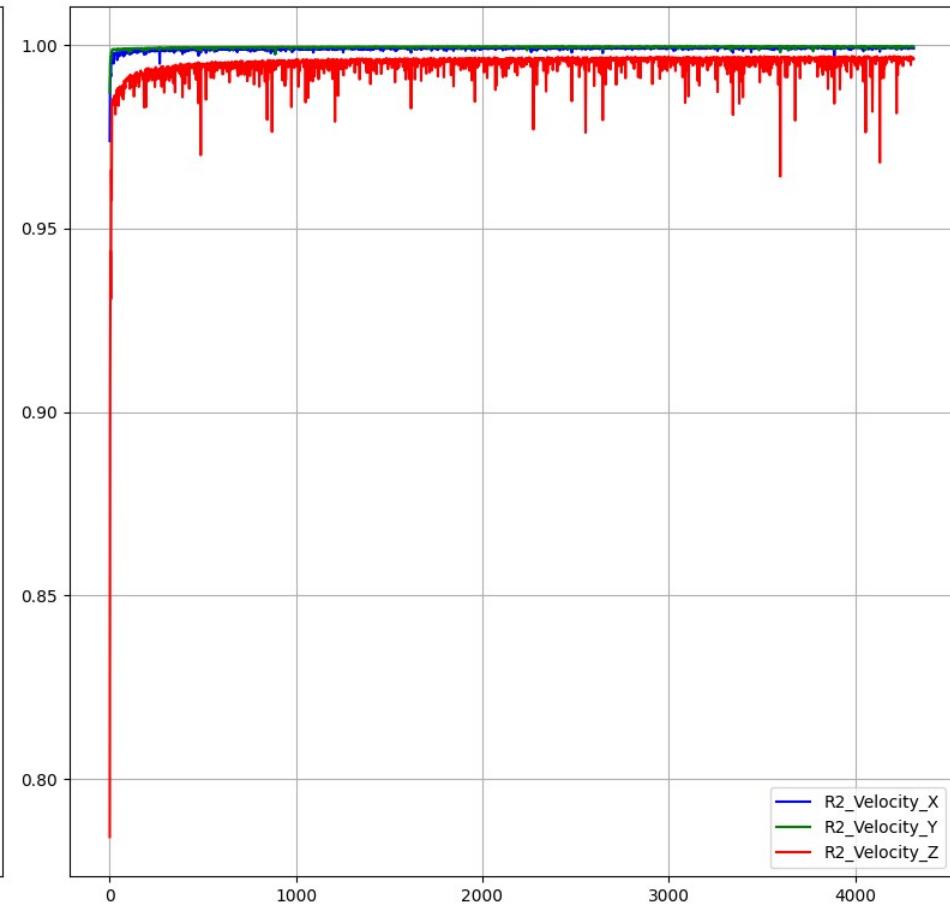


Progress so far - Data + Cont Loss (Adam Optimizer – Std Normal Scalar, Adaptive Weighting)  
Logging Plots (Testing)

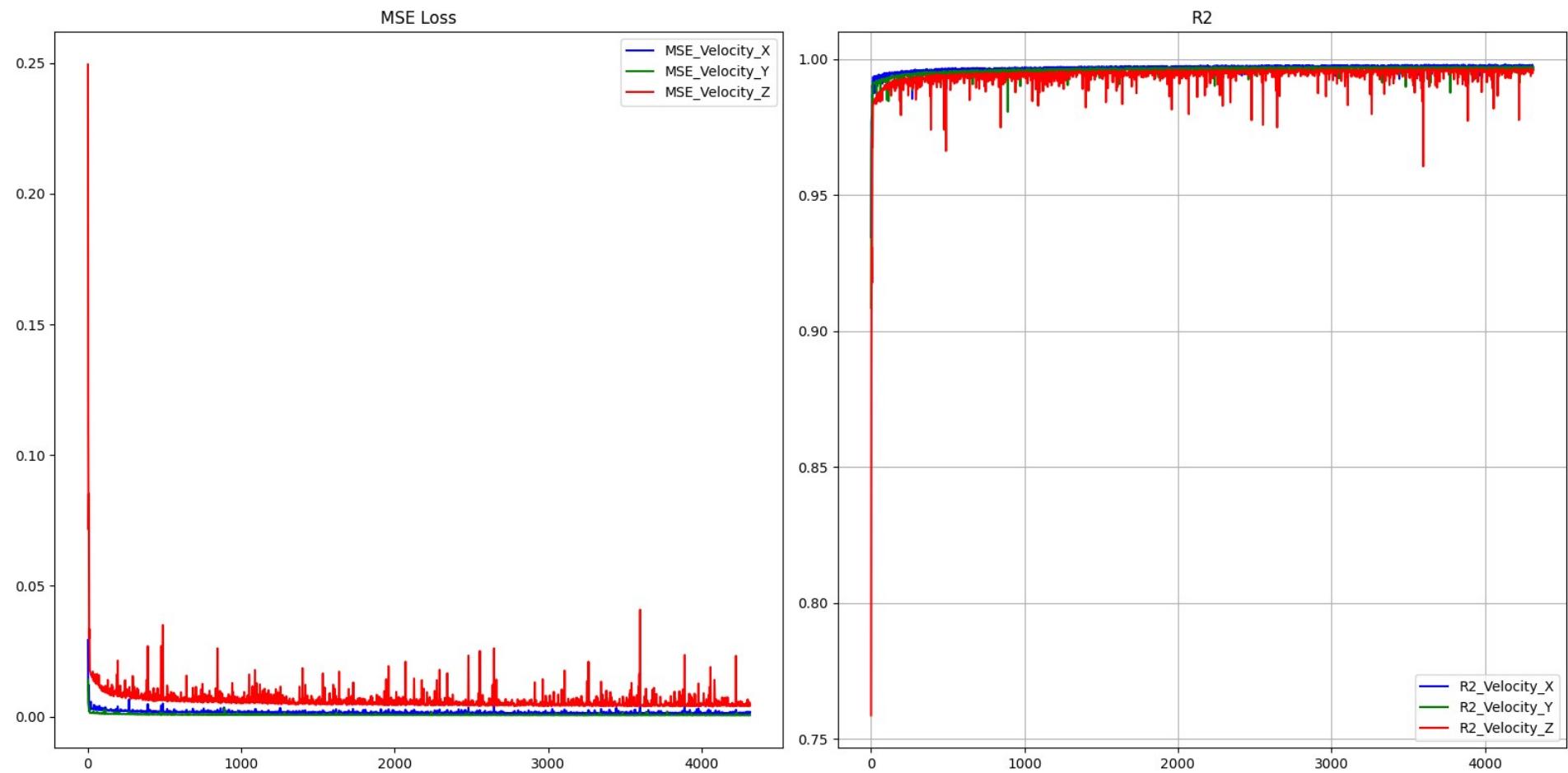
MSE Loss



R2



Progress so far - Data + Cont Loss (Adam Optimizer – Std Normal Scalar, Adaptive Weighting)  
Logging Plots (Predicting 135)



Progress so far - Data + Inlet Loss - Adaptive Weighting

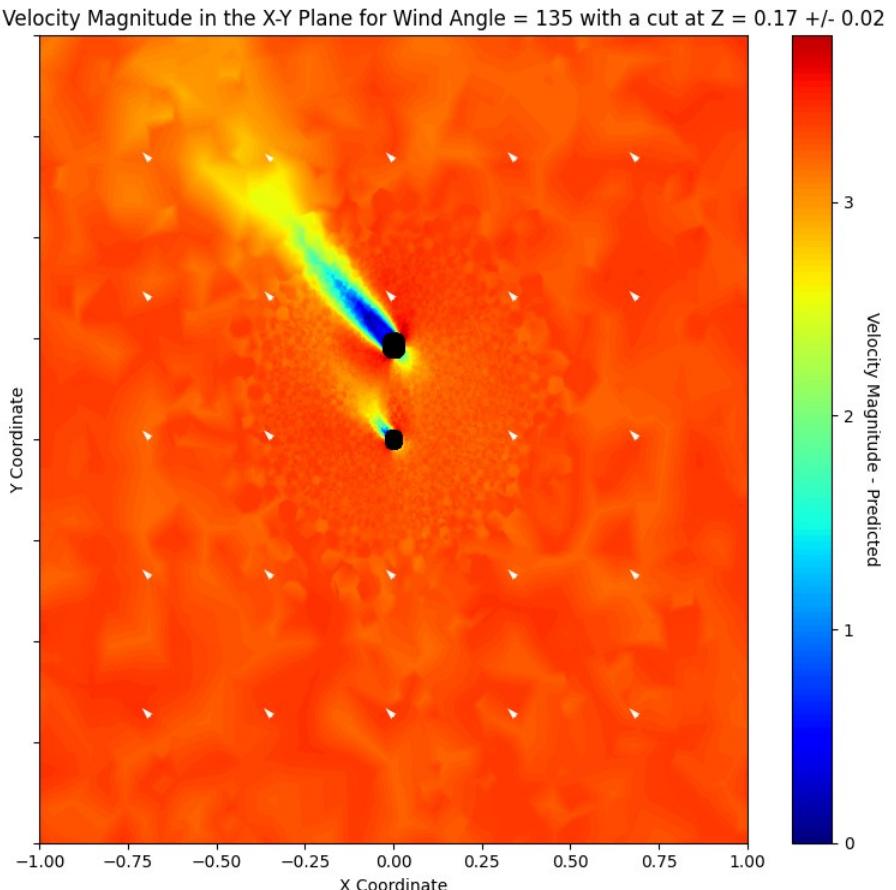
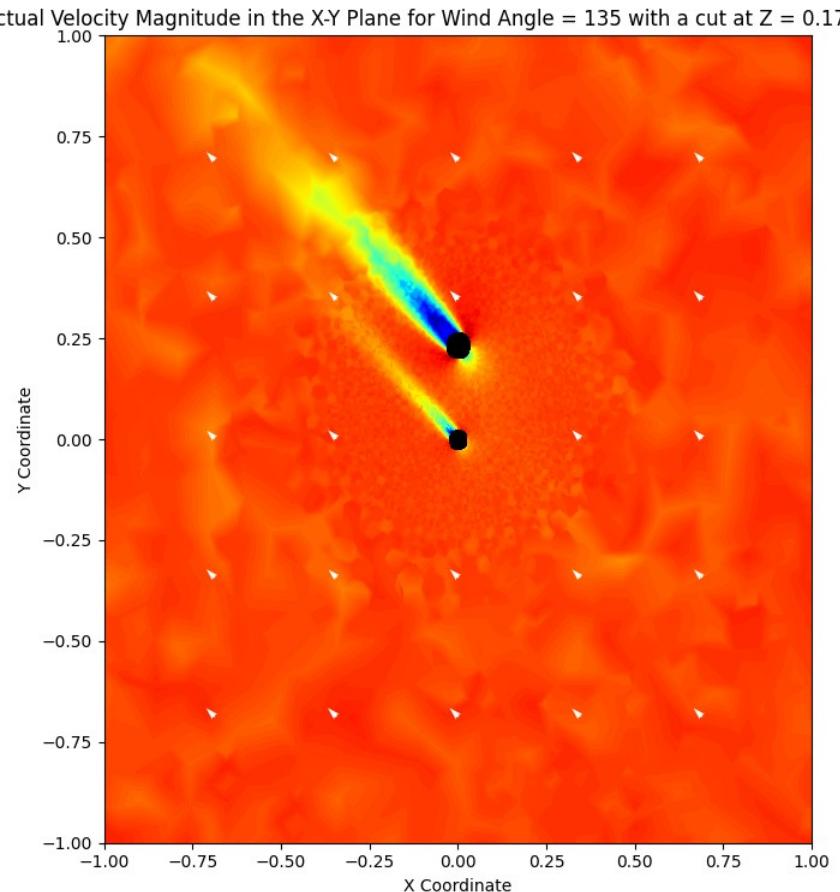
Threshold = SMA1E-5 (4314 Epochs, not completed)

Predicting Results – Metrics (Angle = 135)

Variable	MSE	RMSE	MAE	R2
Velocity:0	0.0039158792740959	0.0625769867770566	0.0515793193738456	0.996157991859468
Velocity:1	0.0031648030142739	0.0562565819640149	0.0380693264974221	0.996924502638539
Velocity:2	0.0001320390879873	0.0114908262534672	0.0066009895744564	0.995963842826592

Progress so far - Data + Cont Loss - Adaptive Weighting  
Threshold = SMA1E-5 (4314 Epochs, not completed)

Comparison of Actual vs. Predicted values with Wind Angle = 135 in the X-Y Plane with a cut at Z = 0.17 +/- 0.02



# Some Next Steps

La Defense